Polyphemus 1.0
User's Guide

CEREA – ENPC / EDF R&D
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Chapter 1

Introduction and Installation

1.1 Polyphemus Overview

Polyphemus is an air-quality modeling system built to manage:

- several scales: local, regional and continental scales;
- many pollutants: from non-reactive species to particulate matter;
- several chemistry-transport models;
- a bunch of advanced methods in data assimilation and ensemble forecasting;
- model integration.

Further details are available in:
Mallet, V., Quélo, D., and Sportisse, B. (2005). Software architecture of an ideal modeling platform in air quality – A first step: Polyphemus. Technical Report 11, CEREA

Polyphemus is made of:

- data processing abilities (available in libraries);
- a library for physical parameterizations (library AtmoData);
- programs to compute input data to chemistry-transport models;
- chemistry-transport models;
- drivers, that is, object-oriented codes responsible for driving models in order to perform, for instance, simulations and data assimilation;
- programs to analyze and display output concentrations (notably based on the library AtmoPy).

Its flowchart is shown in Figure 1.1, in which three steps may be identified: (1) preprocessing (interpolations, physical parameterizations), (2) model computations (possibly with data assimilation or any other method implemented in a driver), (3) postprocessing (comparisons to measurements, statistics, visualization).

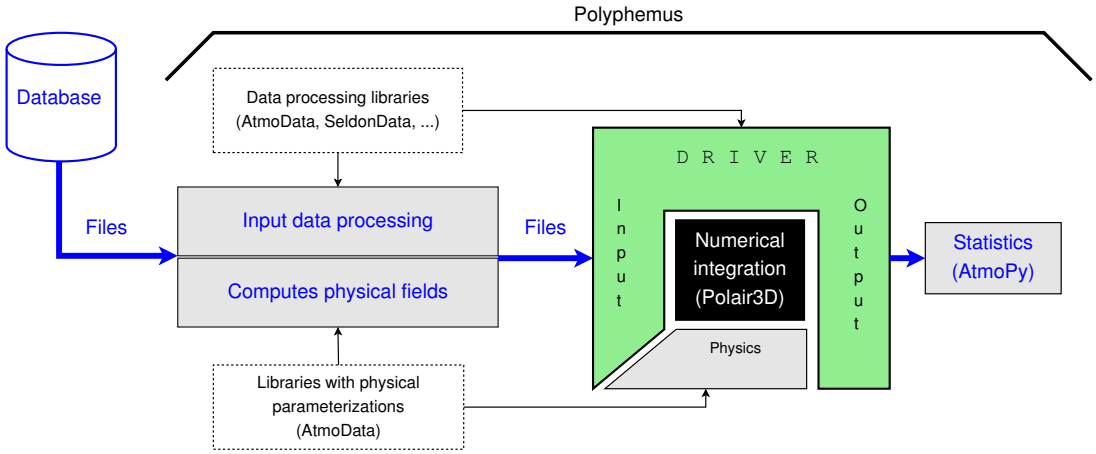


Figure 1.1: Polyphemus flowchart (preprocessing, model computations, postprocessing).

As a consequence, Polyphemus code is organized with the following directories tree:

`preprocessing`

- `bc`: boundary conditions (Mozart 2, Gocart);
- `bio`: biogenic emissions;
- `dep`: deposition velocities;
- `emissions`: pollutant emissions (EMEP);
- `ground`: ground data (land use cover, roughness);
- `ic`: initial conditions (Mozart 2);
- `meteo`: meteorological data (ECMWF and MM5, including cloud attenuation and vertical diffusion);

`driver`: forward simulations, data assimilation;

- `example`: a series of examples of configuration files for several applications;
- `observation`: observation managers for data assimilation (ground observations and simulated observations);
- `output_saver`: modules to save the results of a simulation;

`postprocessing`: comparisons to measurements;

- `water_plume`: liquid water diagnosis in a plume;

`include`

- `Talos`: C++ library to manage configuration files (used everywhere in Polyphemus), dates and string processing;
- `SeldonData`: C++ library to perform data processing (interpolations, input/output operations);
- `AtmoData`: C++ library of physical parameterizations;
- `atmopy`: AtmoPy is a Python library for statistical analysis and visualization;

`common`: some functions used to parse and manage the arguments of preprocessing programs;

`models`: chemistry-transport models to be used by the drivers;

`modules`

`common`: a base module from which transport and chemistry modules derive,

`transport`: numerical schemes for advection and diffusion;

`chemistry`: chemical mechanisms;

`utils`: some useful tools.

Polyphemus is an open source software distributed under the GNU General Public License. It is available at `http://www.enpc.fr/cerea/polyphemus/`. Polyphemus development and support team can be contacted at `polyphemus@cerea.enpc.fr`.

1.2 Requirements

Polyphemus is designed to run under Unix or Linux-based systems. It should be able to run under Windows. AtmoPy has been tested under Windows and Polair3D has been compiled with Microsoft Visual Studio.NET 2003. There is no obvious reason why other parts of Polyphemus should not work under Windows.

Polyphemus is based on three computer languages: C++, Fortran 77 and Python. There are also a very few lines of C.

Supported C++ compilers are GNU GCC (G++) 3.2, 3.3, 3.4, 4.0 and 4.1. GNU GCC 2.x series is too old to compile Polyphemus. Intel C++ compiler (ICC, versions 7.1 and 8.0) should work.

Corresponding Fortran compilers are acceptable: GNU G77 3.2, 3.3 and 3.4, GNU GFORTRAN 4.0 and 4.1, and Intel Fortran compilers IFC 7.1 and IFORT 8.0.

Note for GCC users: Please note that Fortran 77 compiler has changed between version 3.x and version 4.x of GCC and that those two versions are not compatible. In particular, if you choose to use GFORTRAN make sure to use the corresponding C++ compiler and not an older version.

Python supported versions are 2.3 and 2.4.

With regard to software requirements, below is a list of possible requirements (depending on the programs to be run):

- the C++ library Blitz++ (`http://www.oonumerics.org/blitz/`): versions 0.6, 0.7, 0.8 and 0.9 are supported. Note that your compiler may exclude a few versions.
- Blas/Lapack: any recent version.
- NewRan: C++ library for generation of random numbers, from version 2.0.
- NetCDF: C++ library, any version from series 3.x should work.
- Numarray: series 1.x is supported.
- Matplotlib: any recent version and corresponding pylab version (usually, pylab is included in Matplotlib package). It is recommended to install the corresponding version of Basemap in order to benefit from AtmoPy map-visualizations.

- SciPy: any recent version.

All of them are open source software. Requirements are shown in Table 1.1.

NewRan is not included in Table 1.1 because it is only needed if one uses the class `SimObservationManager` with data assimilation drivers.

Table 1.1: Polyphemus requirements.

	Blitz++	Blas/Lapack	NetCDF	Numarray	Matplotlib	SciPy
`driver`	X	X				
`include`						
`/atmopy`				X	X	X
`preprocessing`						
`/bc`	X		X			
`/bio`	X					
`/dep`	X					
`/emissions`	X					
`/ground`	X					
`/ic`	X		X			
`/meteo`	X					
`postprocessing`				X	X	X
`/water_plume`	X					

1.3 Installation

1.3.1 Main instructions

As soon as libraries and compilers are available, Polyphemus is almost installed. First, extract Polyphemus sources to a given directory. Polyphemus is usually distributed in a `.tar`, `.tgz`, `.tar.gz` or `.tar.bz2` file. These files are extracted with one of these commands:

```
tar -xvf Polyphemus.tar
tar -zxvf Polyphemus.tgz
tar -zxvf Polyphemus.tar.gz
tar -jxvf Polyphemus.tar.bz2
```

Polyphemus programs must be compiled by the user when needed. Makefiles are provided so that program compilation should be easy. For instance, one may compile the program `meteo.cpp` in this way:

```
cd Polyphemus/preprocessing/meteo
make meteo
```

Then the program `meteo` is compiled and can be run. Launch `make` in order to compile all programs in a given directory. In directory `driver/`, you may use `scons` instead of `make` if you are familiar with SCons[†1].

[†1] http://www.scons.org/

1.3.2 AtmoPy

A special step is required with the Python library AtmoPy. This library makes calls to a C++ program in order to parse configuration files. Follow the steps below to have AtmoPy fully installed:

```
cd Polyphemus/include/atmopy/talos
g++ -I../../Talos -o extract_configuration extract_configuration.cpp
```

You may replace g++ with any supported compiler (see Section 1.2).

1.3.3 Newran

The library Newran is required with Kalman algorithms (RRSQRT and ensemble) to generate random numbers. It should be installed in `include/newran/`.

Download Newran from `http://www.robertnz.net/download.html` (or type "Newran" in search engine). At the time these lines are written, Newran 3.0 beta is available at `http://www.robertnz.net/ftp/newran03.tar.gz`. The following commands work with Newran 3.0 beta (released 22 April 2006); there may be slight changes with other versions.

Create directory `include/newran/`, expand Newran in it:

```
mkdir Polyphemus/include/newran
cd Polyphemus/include/newran
wget http://www.robertnz.net/ftp/newran03.tar.gz
tar -zxvf newran03.tar.gz
```

If all is fine, you should have a file called `include/newran/newran.h`. Next, you have to edit `include/newran/include.h` and uncomment the line:

```
//#define use_namespace                    // define name spaces
```

That is, remove the first two slashes:

```
#define use_namespace                    // define name spaces
```

Compile the library (here, with GNU C++ compiler):

```
make -f nr_gnu.mak libnewran.a
```

This should create `include/newran/libnewran.a`. To complete the installation, you have to create a directory where the seed values are stored, for instance:

```
mkdir ~/.newran
cp fm.txt lgm.txt lgm_mix.txt mother.txt mt19937.txt multwc.txt wh.txt ~/.newran/
```

Recall the path to your seed directory since this is an entry of a configuration file (`driver/example/assimilation/perturbation.cfg`).

Chapter 2

Using Polyphemus

2.1 Remark

In configurations files, in output logs, and so on, indices start at 0 (as in C++ and Python, not at 1 as in Fortran).

2.2 Configuration Files

2.2.1 Definitions

All Polyphemus programs rely on flexible configuration files. These configuration files define simulation domains, input and output paths, options, etc.

Configurations files are text files, preferably with extension `.cfg`. They primarily contain *fields*, that is, entries associated with *values* provided by the user. In a configuration file, a line usually reads:

```
field = value
```

A practical example is a discretization definition:

```
x_min = 12.5
Delta_x = 0.5
Nx = 100
```

The *fields* `x_min`, `Delta_x` and `Nx` are associated with proper *values* specified by the user.

The characters put between a field and its value are *delimiters*. In the previous example, the delimiters are blank spaces and equal signs. *Delimiters* are discarded characters. They may be put anywhere in a configuration file but they are always ignored. Their aims are to delimit words (i.e., fields and values) and to make the configuration file clearer.

2.2.2 Flexibility

The fields and values can be introduced in many ways. First, many delimiters are supported:

- blank space ( ),
- tabulation (	),
- line break,

- equal sign (=),
- colon (:),
- semicolon (;),
- coma (,), and
- vertical bar (|).

For example,

```
x_min = 12.5
Delta_x = 0.5
Nx = 100
```

is equivalent to

```
x_min 12.5
Delta_x == 0.5
Nx: 100
```

Recall that delimiters can only be used to delimit words, and are discarded otherwise. It means that a field or a value cannot contain a delimiter.

Fields and values go by pair, but they can be placed anywhere. In particular, several fields may be put on a single line:

```
x_min = 12.5    Delta_x = 0.5    Nx = 100
y_min = -6.2    Delta_y = 1.     Ny = 230
```

The order in which the fields are placed may or may not be important. In most Polyphemus configuration files, the order does not matter. Then

```
x_min = 12.5    Delta_x = 0.5    Nx = 100
y_min = -6.2    Delta_y = 1.     Ny = 230
```

is the same as

```
y_min = -6.2    Delta_y = 1.     Ny = 230
Nx = 100        x_min = 12.5     Delta_x = 0.5
```

Recommandation – Use equal sign '=' between a field and its value if the value is a number and use semi-colon ':' if the value is a string. Example:

```
x_min = 12.5
Output_directory: /home/user/path
```

2.2.3 Comments

Comment lines may be added. They start with '#' or with '%':

```
# Path where results are written.
Output_directory: /home/user/path
```

They may also be put at the end of a line:

```
Output_directory: /home/user/path  # Path where results are written.
```

Recommandation – Prefer '#' for comments, so as to be consistent with Polyphemus default configuration files.

2.2.4 Markups

In order to avoid duplications in a configuration file, Polyphemus features a markup management. A markup is denoted with surrounding '<' and '>', e.g. <path>. A markup is automatically replaced with its value whenever it is found. Its value should be provided somewhere in the configuration file with a proper field; for instance, <path> refers to the field path. Here is a complete example:

```
Root: /home/user
Input_directory: <Root>/input/
Output_directory: <Root>/output/
```

means:

```
Input_directory: /home/user/input/
Output_directory: /home/user/output/
```

The markup can be used before its value is defined:

```
Input_directory: <Root>/input/
Output_directory: <Root>/output/
Root: /home/user # After calls to <Root>. This is legal.
```

Any field may be used as a markup. The user may define any new markup (that is a new field). Moreover, several markup substitutions can be performed in a single value, and nested markups are properly handled:

```
Home: /home/user
Root: <Home>/Polyphemus/work
Number = 7
Input_directory: <Root>/input-<Number>/
```

is accepted and means:

```
Input_directory: /home/user/Polyphemus/work/input-7/
```

Notice that markups may also replace numbers and may be based on preexisting fields:

```
x_min = 12.5    Delta_x = 0.5    Nx = 100
y_min = <x_min> Delta_y = 1.     Ny = <Nx>
```

2.2.5 Sections

Fields and values may be protected inside sections. Assume that two domains are defined, one for input data and another for output data. Instead of:

```
x_min_in = 12.5    Delta_x_in = 0.5    Nx_in = 100
x_min_out = 35.8   Delta_x_out = 0.3   Nx_out = 400
```

one may prefer:

```
[input]
x_min = 12.5    Delta_x = 0.5    Nx = 100

[output]
x_min = 35.8    Delta_x = 0.3    Nx = 400
```

Conflicts are avoided and the syntax is clear. This is why most Polyphemus configuration files have sections.

Sections are enclosed by square brackets ('[' and ']').

Markups are not bound to any section.

Recommandation – Put two blank lines before each section and one blank line after:

```
( blank line )
( blank line )
[input]
( blank line )
x_min = 12.5    Delta_x = 0.5    Nx = 100


[output]

x_min = 12.5    Delta_x = 0.5    Nx = 100
```

2.2.6 Multiple Files

Several Polyphemus programs accept two configuration files as input. Providing two configuration files is then equivalent to providing a single configuration file that would contain all the lines of both files. This is useful to let several programs share a same configuration base. For instance, the simulation domain (whose description is needed by most programs) is usually defined in a configuration file that is provided to every program, in addition to a file dedicated to the specific configuration of the program.

For instance:

```
./emissions general.cfg emissions.cfg 20010506
```

launches the program `emissions` with two configuration files as input: (1) the configuration file `general.cfg` shared with other programs and notably defining the domain description, (2) a specific configuration file, `emissions.cfg`, that includes options for emission generation.

Markups defined in one configuration file can be used in the other file. Note however that each section must be defined in one file only.

2.2.7 Dates

Date formats are:

```
YYYY                # Year.
YYYY-MM             # With the month.
YYYY-MM-DD          # With the day.
YYYY-MM-DD_HH       # With the hour.
YYYY-MM-DD_HH-II    # With the minute.
YYYY-MM-DD_HH-II-SS # With the second.
```

Months range from `01` to `12`. Days range from `01` to `31`. Hours range from `00` to `23`. Minutes and seconds range from `00` to `59`.

If the month is not specified (format `YYYY`), then the month is set to `01` (January). If the day is not specified (formats `YYYY` and `YYYY-MM`), it is set to `01` (first day of the month). If the hour, the minute or the second is not specified, it is set to zero (`00`).

Hyphens and underscores may be replaced with any character that is neither a delimiter (see Section 2.2.2) nor a cipher. They can also be removed. Examples:

```
19960413
1996-04-13_20h30
1996/04/13@2030
```

Recommandation – Use hyphens around the month and around minutes. Use an underscore between the day and the hour (`YYYY-MM-DD_HH-II-SS`).

2.2.8 Booleans

Booleans are supported in configuration files and can be specified in any of the following ways:

```
true   t   yes   y
false  f   no    n
```

This is case unsensitive: e.g., `True` or `NO` are valid.

2.3 Running Programs

2.3.1 Compiling Programs

Along with all programs are provided makefiles, in the same directory. Edit these makefiles to change the compiler. Main variables are the C++ compiler `CC`, the Fortran compiler `F77`, the linker `LINK`, and maybe the libraries `LIBS` and the include paths `INCPATH`.

2.3.2 Running a Program

Most programs require one or two input configuration-files, and sometimes a date. Most programs provide help when launched without any input file. Here is an example with the program `meteo`[†1]:

```
~/Polyphemus/preprocessing/meteo/> ./meteo

Usage:
   ./meteo [main configuration file] [secondary configuration file] [date]
   ./meteo [main configuration file] [date]
   ./meteo [date]

Arguments:
  [main configuration file] (optional): main configuration file. Default: meteo.cfg
  [secondary configuration file] (optional): secondary configuration file.
  [date]: date in format YYYYMMDD.
```

Program `meteo` takes from one to three arguments. Below are three possible calls:

[†1] Further details about specific programs are provided in chapter 3.

```
./meteo 20010422
./meteo meteo.cfg 20010422
./meteo ../general.cfg meteo.cfg 20010422
```

The first line is equivalent to `meteo meteo.cfg 20010422`. The third line involves two configuration files. The program `meteo` behaves as if these two configuration files were merged. It means that the fields required by the program may be put in any of these two files. Markups defined in one file can be expanded in the other file. The only constraint is that each section should appear in a single file only.

2.3.3 Sharing Configuration

The command line:

```
./meteo ../general.cfg meteo.cfg 20010422
```

with the two configuration files `general.cfg` and `meteo.cfg`, is the advocated line. The configuration file `general.cfg` gathers information that may be needed by several programs in the `preprocessing` directory (`meteo`, `attenuation`, `luc-usgs`, etc.). Such a configuration file is provided with `Polyphemus/preprocessing/general.cfg`:

```
[general]

Home: /u/cergrene/0/bordas
Directory_computed_fields: <Home>/B/data
Directory_ground_data: <Directory_computed_fields>/ground
Programs: <Home>/codes/Polyphemus-HEAD


[domain]

Date: 20010422
t_min = 0.0     Delta_t = 3.0   Nt = 9
x_min = -10.0   Delta_x = 0.5   Nx = 65
y_min = 40.5    Delta_y = 0.5   Ny = 33
Nz = 5
Vertical_levels: <Programs>/levels.dat
```

The simulation domain and the simulation dates are defined. In addition, markups (`Directory_computed_fields`, `Directory_ground_data` and `Programs`) are introduced and may be referred by other configuration files such as `meteo.cfg`.

Actually most configuration files (`meteo.cfg`, `luc-usgs.cfg`, `emissions.cfg`, etc.) provided in Polyphemus, along with the programs, are examples that refer to the markups defined in `general.cfg`. Essentially three markups are defined in `general.cfg`:

- `Directory_computed_fields`: where output results (i.e., fields computed by preprocessing programs) are stored.
- `Directory_ground_data`: where ground data (land use cover, roughness) is stored.
- `Programs`: path to Polyphemus preprocessing directory.

Polyphemus configuration files are written so that mainly changes in `general.cfg` should be needed to perform a reference simulation. In `general.cfg`, one changes the paths (markups) to the programs (`Programs`) and to the output results (`Directory_computed_fields` and `Directory_ground_data`), and one chooses its simulation domain. Other configuration files provide paths to input data (meteorological files, emissions data, etc.) and fine options.

2.3.4 Notes about Models

To launch a simulation you have to compile and execute a C++ program which differs from preprocessing programs. After preprocessing steps, the simulation is made of a driver (on top of the model itself), a model and its modules (if any). See Section 1.1 for a short description of the flowchart. The program of the simulation looks like `driver/polair3d.cpp`: it is a short C++ code that declares the driver, the model and the modules.

You may have to modify this program in case you change the model, the driver or a module. In that case, duplicate `driver/polair3d.cpp` (or another example) and modify it according to the notes below. Actually it is likely that the model/driver combination is already in use in one of the examples: have a look in `driver/*.cpp`.

First determine which model you need, depending on your simulation target:

- for a passive simulation: `Polair3DTransport` or `CastorTransport`;
- for a simulation with chemistry for gaseous species: `Polair3DChemistry` or `CastorChemistry`;
- for a simulation with aerosol species: `Polair3DAerosol`;
- for a simulation with gaseous species and data assimilation: `Polair3DChemistryAssimConc`;
- for a simulation at local scale using an Eulerian model: one of Polair3D models with driver `StationaryDriver`;
- for a simulation with a plume Gaussian model: `GaussianPlume`, or `GaussianPlume_aer` if there are aerosol species;
- for a non-stationary simulation at local scale with a Gaussian model: `GaussianPuff`, or `GaussianPuff_aer` if there are aerosol species.

To set the model, just modify the definition of `ClassModel`:

```
typedef MyModel<Argument(s)> ClassModel;
```

For instance:

```
typedef Polair3DAerosol<real, AdvectionDST3<real>,
    DiffusionROS2<real>, Decay<real> > ClassModel;
```

If you change a model, you may also change the modules (a model may need less modules or no module at all: remove them is necessary). The modules are all (template) arguments of the model (`AdvectionDST3<real>`, `DiffusionROS2<real>` and `Decay<real>`, in the previous example), except for `real` that should not be changed. The order in which the modules are provided matters: it is always advection, diffusion and chemistry, or transport (single module) and chemistry. See Section 2.5.5 for the modules you can use with the model you chose.

Then, in your main C++ program, declare the right driver. You may replace `BaseDriver` with a new driver at this line (in `driver/polair3d.cpp`):

```
BaseDriver<real, ClassModel, BaseOutputSaver<real, ClassModel> >
  Driver(argv[1]);
```

Finally make sure to include all models, modules, drivers and output savers you use (at the beginning of the file – statements `#include "...cxx"`). The makefile may need changes too if the module uses Fortran functions. In particular, chemistry modules `ChemistryRADM` and `ChemistryRACM` need Fortran routines, make sure that they are included in `SRC77`:

- for `ChemistryRACM`: LU_decompose.f, LU_solve.f, angzen.edf.f, chem.f, dratedc.f, fexchem.f, jacdchemdc.f, kinetic.f, rates.f, roschem.f and solvlin.f (in directory `include/modules/chemistry/ChemistryRACM`).
- for `ChemistryRADM`: LU_decompose.f, LU_solve.f, angzen.edf.f, chem.f, fexchem.f, jacdchemdc.f, kinetic.f, roschem.f and solvlin.f (in directory `include/modules/chemistry/ChemistryRADM`).

Chemistry module `ChemistryRACM-SIREAM` also needs Fortran routines, but a specific makefile is provided for simulations using this module.

If you are not confident with your own changes, have a look at the examples: it is likely that you find a close combination there. In case you try an unusual combination, you may contact `polyphemus@cerea.enpc.fr`.

The directory named `driver/example` provides examples of configuration and data files to use with the programs. These examples should be launched *in* directory `driver`. Their outputs will then be stored in `driver/results`, so make sure that this directory exists **before** you start the simulation (indeed Polyphemus programs do not create directories before saving results).

2.4 Useful Tools

A few useful tools are provided in directory `Polyphemus/utils`. Here is a brief explanation of their aim and their use.

2.4.1 Information about Binary Files

Two programs provided in `Polyphemus/utils` are meant to provide information about the content of binary files. It is highly recommended to use these programs to check the output files of preprocessing programs and drivers/models (e.g. in Section 2.5.6).

These two programs perform the same thing but on binary files with different floating precision:

- `get_info_float` gives the minimum, maximum and mean of a binary file in single precision.
- `get_info_double` gives the minimum, maximum and mean of a binary file in double precision.

It is assumed that the binary file to be analyzed by `get_info_float` or `get_info_double`, contains only floating point numbers. No extra data such as headers should be in the file. Output binary files from preprocessing programs and from drivers/models satisfy this condition and can be properly read by `get_info_float` or `get_info_double`. Note that Polyphemus programs usually generate single precision files: it is very likely that one only uses `get_info_float`.

Using `get_info_float` or `get_info_double` is straightforward:

```
$ get_info_float Temperature.bin

Minimum: 257.621
Maximum: 300.882
Mean: 282.262

$ get_info_float Temperature.bin Pressure.bin

-- File "Temperature.bin"
Minimum: 257.621
Maximum: 300.882
Mean: 282.262

-- File "Pressure.bin"
Minimum: 56369.2
Maximum: 102496
Mean: 87544.1
```

2.4.2 Differences between Two Binary Files

There are two different types of programs to compute statistics about the differences between two files:

- `get_diff_precision` where `precision` is `float` or `double`. They return statistics about the difference between two files. As for `get_info_precision`, the files should only contain floating point numbers.

- `get_partial_diff_precision` where `precision` is `float` or `double`. They return statistics about the difference between two files. If these two files have the same size, `get_partial_diff_precision` does the same as `get_diff_precision`. If the files do not have the same size, only the first values (as much as possible) are compared.

Here is an example with `get_diff_float`:

```
~Polyphemus/driver/results> ../../utils/get_diff_float O3.bin O3-other.bin

                File #0         File #1
Minima:         0.0145559       0.0181665
Maxima:         136.795         175.123
Means:          71.578          65.4088
Standard dev.:  26.958          28.643

                Difference
Minimum:        -57.324
Maximum:        66.9219
Mean:           6.16919
Standard dev.:  14.4999

Correlation between files #0 and #1: 0.865696
```

2.4.3 MM5 Files

It can be useful to get information from MM5 file, in particular to modify the configuration file `MM5-meteo.cfg` (see Section 3.4.5). To do so, two programs are provided:

- `MM5_var_list` gives a list of all variables stored in a MM5 file. It also gives miscellaneous information about the file. Information provided can be needed in preprocessing step (program `MM5-meteo` – Section 3.4.5): number of space steps, time step and projection type.
- `get_info_MM5` gives the minimum, maximum, mean and standard deviation of a variable stored in a MM5 file (use program `MM5_var_list` to know what variables are stored in the file).

For instance, the output of `MM5_var_list` for the file `MM5-2004-08-09` used in the Eulerian test case (see Section A) is:

```
Metadata (-999 means unknown):

OUTPUT FROM PROGRAM MM5 V3 : 11
TERRAIN VERSION 3 MM5 SYSTEM FORMAT EDITION NUMBER : 1
TERRAIN PROGRAM VERSION NUMBER : 6
TERRAIN PROGRAM MINOR REVISION NUMBER : 0
COARSE DOMAIN GRID DIMENSION IN I (N-S) DIRECTION : 76
COARSE DOMAIN GRID DIMENSION IN J (E-W) DIRECTION : 86
MAP PROJECTION. 1: LAMBERT CONFORMAL, 2: POLAR STEREOGRAPHIC, 3: MERCATOR : 1
IS COARSE DOMAIN EXPANDED?, 1: YES, 0: NO : 0
EXPANDED COARSE DOMAIN GRID DIMENSION IN I DIRECTION : 76
EXPANDED COARSE DOMAIN GRID DIMENSION IN J DIRECTION : 86
GRID OFFSET IN I DIR DUE TO COARSE GRID EXPANSION : 0
GRID OFFSET IN J DIR DUE TO COARSE GRID EXPANSION : 0
DOMAIN ID : 1
MOTHER DOMAIN ID : 1
NEST LEVEL (0: COARSE MESH) : 0
DOMAIN GRID DIMENSION IN I DIRECTION : 76
DOMAIN GRID DIMENSION IN J DIRECTION : 86
I LOCATION IN THE MOTHER DOMAIN OF THE DOMAIN POINT (1,1) : 1
J LOCATION IN THE MOTHER DOMAIN OF THE DOMAIN POINT (1,1) : 1
DOMAIN GRID SIZE RATIO WITH RESPECT TO COARSE DOMAIN : 1
                                                     : 1
REGRID Version 3 MM5 System Format Edition Number : 2
REGRID Program Version Number : 16
REGRID Program Minor Revision Number : 1
COARSE DOMAIN GRID DISTANCE (m) : 36000
COARSE DOMAIN CENTER LATITUDE (degree) : 47
COARSE DOMAIN CENTER LONGITUDE (degree) : 6
CONE FACTOR : 0.715567
TRUE LATITUDE 1 (degree) : 60
TRUE LATITUDE 2 (degree) : 30
POLE POSITION IN DEGREE LATITUDE : 90
APPROX EXPANSION (m) : 360000
```

```
GRID DISTANCE (m) OF THIS DOMAIN : 36000
I LOCATION IN THE COARSE DOMAIN OF THE DOMAIN POINT (1,1) : 1
J LOCATION IN THE COARSE DOMAIN OF THE DOMAIN POINT (1,1) : 1
I LOCATION IN THE COARSE DOMAIN OF THE DOMAIN POINT (IX,JX) : 76
J LOCATION IN THE COARSE DOMAIN OF THE DOMAIN POINT (IX,JX) : 86
TERRAIN DATA RESOLUTION (in degree) : 0.0833333
LANDUSE DATA RESOLUTION (in degree) : 0.0833333

MM5 Version 3 MM5 System Format Edition Number : 1
MM5 Program Version Number : 6
MM5 Program Minor Revision Number : 1
FOUR-DIGIT YEAR OF START TIME : 2004
INTEGER MONTH OF START TIME : 8
DAY OF THE MONTH OF THE START TIME : 9
HOUR OF THE START TIME : 0
MINUTES OF THE START TIME : 0
SECONDS OF THE START TIME : 0
TEN THOUSANDTHS OF A SECOND OF THE START TIME : 0
MKX: NUMBER OF LAYERS IN MM5 OUTPUT : 25
TIMAX:   SIMULATION END TIME (MINUTES) : 5760
TISTEP:  COARSE-DOMAIN TIME STEP IN SECONDS : 100
TAPFRQ:  TIME INTERVAL (MINUTES) THAT DATA WERE SAVED FOR GRIN : 60

Outputs:

Name      Dim. 1   2   3   4   Stag. Ord. Units            Description
U         3    76  86  25      D     YXS  m/s              U COMPONENT OF
                                                           HORIZONTAL WIND
V         3    76  86  25      D     YXS  m/s              V COMPONENT OF
                                                           HORIZONTAL WIND
T         3    76  86  25      C     YXS  K                TEMPERATURE
Q         3    76  86  25      C     YXS  kg/kg            MIXING RATIO
CLW       3    76  86  25      C     YXS  kg/kg            CLOUD WATER MIXING RATIO
RNW       3    76  86  25      C     YXS  kg/kg            RAIN WATER MIXING RATIO
ICE       3    76  86  25      C     YXS  kg/kg            CLOUD ICE MIXING RATIO
SNOW      3    76  86  25      C     YXS  kg/kg            SNOW MIXING RATIO
GRAUPEL   3    76  86  25      C     YXS  kg/kg            GRAUPEL MIXING RATIO
RAD TEND  3    76  86  25      C     YXS  K/DAY            ATMOSPHERIC RADIATION TENDENCY
W         3    76  86  26      C     YXW  m/s              VERTICAL WIND COMPONENT
PP        3    76  86  25      C     YXS  Pa               PRESSURE PERTURBATION
PSTARCRS  2    76  86          C     YX   Pa               (REFERENCE) SURFACE PRESSURE
                                                           MINUS PTOP
GROUND T  2    76  86          C     YX   K                GROUND TEMPERATURE
RAIN CON  2    76  86          C     YX   cm               ACCUMULATED CONVECTIVE
                                                           PRECIPITATION
RAIN NON  2    76  86          C     YX   cm               ACCUMULATED NONCONVECTIVE
                                                           PRECIPITATION
TERRAIN   2    76  86          C     YX   m                TERRAIN ELEVATION
MAPFACCR  2    76  86          C     YX   (DIMENSIONLESS)  MAP SCALE FACTOR
```

```
MAPFACDT  2   76  86        D    YX  (DIMENSIONLESS)  MAP SCALE FACTOR
CORIOLIS  2   76  86        D    YX  1/s              CORIOLIS PARAMETER
RES TEMP  2   76  86        C    YX  K                INFINITE RESERVOIR SLAB
                                                      TEMPERATURE
LATITCRS  2   76  86        C    YX  DEGREES          LATITUDE (SOUTH NEGATIVE)
LONGICRS  2   76  86        C    YX  DEGREES          LONGITUDE (WEST NEGATIVE)
LAND USE  2   76  86        C    YX  category         LANDUSE CATEGORY
TSEASFC   2   76  86        C    YX  K                SEA SURFACE TEMPERATURE
PBL HGT   2   76  86        C    YX  m                PBL HEIGHT
REGIME    2   76  86        C    YX  (DIMENSIONLESS)  PBL REGIME
SHFLUX    2   76  86        C    YX  W/m^2            SENSIBLE HEAT FLUX
LHFLUX    2   76  86        C    YX  W/m^2            LATENT HEAT FLUX
UST       2   76  86        C    YX  m/s              FRICTIONAL VELOCITY
SWDOWN    2   76  86        C    YX  W/m^2            SURFACE DOWNWARD SHORTWAVE
                                                      RADIATION
LWDOWN    2   76  86        C    YX  W/m^2            SURFACE DOWNWARD LONGWAVE
                                                      RADIATION
SWOUT     2   76  86        C    YX  W/m^2            TOP OUTGOING SHORTWAVE
                                                      RADIATION
LWOUT     2   76  86        C    YX  W/m^2            TOP OUTGOING LONGWAVE
                                                      RADIATION
SOIL T 1  2   76  86        C    YX  K                SOIL TEMPERATURE IN LAYER  1
SOIL T 2  2   76  86        C    YX  K                SOIL TEMPERATURE IN LAYER  2
SOIL T 3  2   76  86        C    YX  K                SOIL TEMPERATURE IN LAYER  3
SOIL T 4  2   76  86        C    YX  K                SOIL TEMPERATURE IN LAYER  4
SOIL M 1  2   76  86        C    YX  m^3/m^3          TOTAL SOIL MOIS IN LYR  1  4
SOIL M 2  2   76  86        C    YX  m^3/m^3          TOTAL SOIL MOIS IN LYR  2  4
SOIL M 3  2   76  86        C    YX  m^3/m^3          TOTAL SOIL MOIS IN LYR  3  4
SOIL M 4  2   76  86        C    YX  m^3/m^3          TOTAL SOIL MOIS IN LYR  4  4
SOIL W 1  2   76  86        C    YX  m^3/m^3          SOIL LQD WATER IN LYR  1   4
SOIL W 2  2   76  86        C    YX  m^3/m^3          SOIL LQD WATER IN LYR  2   4
SOIL W 3  2   76  86        C    YX  m^3/m^3          SOIL LQD WATER IN LYR  3   4
SOIL W 4  2   76  86        C    YX  m^3/m^3          SOIL LQD WATER IN LYR  4   4
CANOPYM   2   76  86        C    YX  m                CANOPY MOISTUR E CONTENT
WEASD     2   76  86        C    YX  mm               WATER EQUIVALENT SNOW DEPTH
SNOWH     2   76  86        C    YX  m                PHYSICAL SNOW DEPTH
SNOWCOVR  2   76  86        C    YX  fraction         FRACTIONAL SNOW COVER
ALB       2   76  86        C    YX  fraction         ALBEDO
GRNFLX    2   76  86        C    YX  W m{-2}          GROUND HEAT FLUX
VEGFRC    2   76  86        C    YX  fraction         VEGETATION COVERAGE
SEAICE    2   76  86        C    YX  (DIMENSIONLESS)  SEA ICE FLAG
SFCRNOFF  2   76  86        C    YX  mm               SURFACE RUNOFF
UGDRNOFF  2   76  86        C    YX  mm               UNDERGROUND RUNOFF
T2        2   76  86        C    YX  K                2-meter Temperature
Q2        2   76  86        C    YX  kg kg{-1}        2-meter Mixing Ratio
U10       2   76  86        C    YX  m s{-1}          10-meter U Component
V10       2   76  86        C    YX  m s{-1}          10-meter V Component
ALBD      2   27  2               CA  PERCENT          SURFACE ALBEDO
SLMO      2   27  2               CA  fraction         SURFACE MOISTURE AVAILABILITY
```

```
SFEM      2    27  2                CA   fraction          SURFACE EMISSIVITY AT 9 um
SFZ0      2    27  2                CA   cm                SURFACE ROUGHNESS LENGTH
THERIN    2    27  2                CA   100*cal cm^-2
                                           K^-1 s^1/2        SURFACE THERMAL INERTIA
SFHC      2    27  2                CA   J m^-3 K^-1       SOIL HEAT CAPACITY
SCFX      1    27                   CA   fraction          SNOW COVER EFFECT
SIGMAH    1    25             H     S    sigma             VERTICAL COORDINATE

Total number of time steps read in the file: 97
```

For each variable is provided:

- its name;
- its number of dimensions;
- its length along dimension 1 (if applicable);
- its length along dimension 2 (if applicable);
- its length along dimension 3 (if applicable);
- its length along dimension 4 (if applicable);
- the position at which the variable is given (`Stag.`): dot points (`D`, corner of the grid squares) or cross points (`C`, center of the grid squares);
- its dimensions ordering;
- its unit (or `(DIMENSIONLESS)`);
- a short description.

Then you can use the program `get_info_MM5` to have statistical data about one of the variables only. Note that some variables have a blank space in their name so in that case you need to put the name between quotes to use `get_info_MM5`. If the name has no blank spaces, quotes are not necessary but can be used.

```
~/TestCase/raw_data/MM5> get_info_MM5 MM5-2004-08-09 'GROUND T'

Min: 271.911
Max: 327.747
Mean: 294.112
Std. dev.: 6.46779

~/TestCase/raw_data/MM5> get_info_MM5 MM5-2004-08-09 ALB

Min: 0.0738
Max: 0.8
Mean: 0.122658
Std. dev.: 0.0501975
```

2.4.4 Script `call_dates`

The script `call_dates` allows to call a program (in particular for preprocessing) over several consecutive days. Launch it without arguments to get help:

```
~/Polyphemus/utils> ./call_dates

Script "call_dates" calls a program over a range of dates.
Usage:
  "call_dates" [program] {arguments} [first date] [second date / number of days]
Arguments:
  [program]: program to be launched over the range of dates.
  {arguments}: arguments. Any occurence of %D is replaced with the date;
               otherwise the date is assumed to be the last argument.
  [first date]: first date of the range of dates.
  [second date / number of days]: last date of the range of dates
                                  or number of days of this range.
```

Below is an example:

```
~/Polyphemus/utils> call_dates echo "Current date:" 20060720 20060722

--------------------------------------------------------------------------------
nice time echo Current date: 20060720
Current date: 20060720
0.00user 0.00system 0:00.00elapsed 0%CPU (0avgtext+0avgdata 0maxresident)k
0inputs+0outputs (0major+176minor)pagefaults 0swaps
--------------------------------------------------------------------------------
nice time echo Current date: 20060721
Current date: 20060721
0.00user 0.00system 0:00.00elapsed 0%CPU (0avgtext+0avgdata 0maxresident)k
0inputs+0outputs (0major+177minor)pagefaults 0swaps
--------------------------------------------------------------------------------
nice time echo Current date: 20060722
Current date: 20060722
0.00user 0.00system 0:00.00elapsed 200%CPU (0avgtext+0avgdata 0maxresident)k
0inputs+0outputs (0major+177minor)pagefaults 0swaps
--------------------------------------------------------------------------------
```

For each day, the command that is launched is shown (note that `nice time` has been prepended) and its output is displayed below.

2.5 Setting Up a Simulation

This section is a quick overview of how a simulation should be set up. It is not meant to and cannot replace the chapters about preprocessing, models, modules, ...

2.5.1 Suggested Directory Tree

It is advocated not to modify Polyphemus code, including the configuration files provided with it. The whole Polyphemus directory should not be modified (except maybe makefiles). Copy

the configuration files you need in a dedicated directory, modify the new configuration files in this directory, and run Polyphemus programs from this directory. Your directory tree may look like:

```
Polyphemus-{version}/driver/
                    /include/
                    /postprocessing/
                    /preprocessing/
                    /utils/
MyStudy/configuration/
       /data/emissions/
            /meteo/
            /[...]
       /results/reference/
               /new_emissions/
               /[...]
```

where `MyStudy` contains Polyphemus configurations files set for the study (`configuration` with `general.cfg`, `meteo.cfg`, ... in it), data generated by preprocessing programs (directory `data`), and output results from the chemistry-transport model (`results`, with results from different runs).

Notice that Polyphemus directory includes the version number (or the date). This is very useful in order to properly track simulations. In directory `MyStudy`, you should add a file called `version` which should contain Polyphemus version (and maybe the version of other tools).

You may also want to copy configuration files in your output directory. For instance, you may copy `meteo.cfg` in directory `MyStudy/data/meteo/` so as to know with which configuration your meteorological data were generated.

2.5.2 Roadmaps

Roadmaps with Eulerian Models

In short, the main steps to set up an Eulerian simulation are:

1. generation of ground data (land use cover, roughness height) – `preprocessing/ground`;
2. preprocessing of meteorological fields – `preprocessing/meteo`;
3. other preprocessing steps if relevant (deposition velocities, emissions, ...);
4. compiling the right combination of model, module(s) and driver (see Sections 2.5.5 and 2.3.4).

Passive tracer Below is a possible sequence of programs to be launched to perform a basic passive simulation:

```
preprocessing/ground/luc-glcf
preprocessing/ground/roughness
preprocessing/meteo/MM5-meteo
preprocessing/meteo/Kz_TM
driver/polair3d-transport
```

Program `polair3d-transport` is not provided with Polyphemus. It should be built with Polyphemus components: `BaseDriver` (driver), `Polair3DTransport` (model), `AdvectionDST3` (module), `DiffusionROS2` (module). See Section 2.3.4 for details.

Photochemistry Below is a possible sequence of programs to be launched to perform a photochemistry simulation:

```
preprocessing/ground/luc-glcf
preprocessing/ground/roughness
preprocessing/meteo/MM5-meteo
preprocessing/meteo/Kz_TM
preprocessing/emissions/emissions
preprocessing/bio/bio
preprocessing/dep/dep
preprocessing/ic/ic
preprocessing/bc/bc
driver/polair3d
```

Roadmaps with Gaussian Models

In short, the main steps to set up a Gaussian simulation are:

1. generation of meteorological data: no program is available to do it, but as only little information is required this should be quite easy. Examples of meteorological files are provided in `driver/example/gaussian/gaussian-meteo.dat` and `driver/example/gaussian/gaussian-meteo_aer.dat`.

2. preprocessing: `discretization` to generate source files and `gaussian-deposition` or `gaussian-deposition_aer` to compute deposition velocities (without or with aerosol species respectively). For more details, see Section 3.9

3. compiling the right combination of model (`GaussianPlume`, `GaussianPlume_aer`, `GaussianPuff`, `GaussianPuff_aer`) and driver (`PlumeDriver` or `PuffDriver`).

2.5.3 Mandatory Data in Preprocessing

ECMWF Fields

In ECMWF files, it is recommended to have the following fields (with their Grib codes):

- Volumetric soil water layer 1 (39),
- Volumetric soil water layer 2 (40),
- Volumetric soil water layer 3 (41),
- Volumetric soil water layer 4 (42),
- Temperature [3D] (130),
- U velocity [3D] (131),
- V velocity [3D] (132),
- Specific humidity [3D] (133),
- Snow depth (141),
- Stratiform precipitation (Large-scale precipitation) [accumulated] (142),

- Convective precipitation [accumulated] (143),
- Snowfall (convective + stratiform) [accumulated] (144),
- Surface sensible heat flux [accumulated] (146),
- Surface latent heat flux [accumulated] (147),
- Logarithm of surface pressure (152),
- Boundary layer height (159),
- Total cloud cover (164),
- 2 meter temperature (167),
- Surface solar radiation downwards [accumulated] (169),
- Surface solar radiation [accumulated] (176),
- East-West surface stress [accumulated] (180),
- North-South surface stress [accumulated] (181),
- Evaporation [accumulated] (182),
- Low cloud cover (186),
- Medium cloud cover (187),
- High cloud cover (188),
- Skin temperature (235),
- Forecast albedo (243),
- Cloud liquid water content [3D] (246),
- Cloud ice water content [3D] (247),
- Cloud cover [3D] (248).

Not all data may be required, depending on the programs you actually run.

2.5.4 Mandatory Data for Models

The table below presents all variables needed by various models (and the name under which they appear in the data configuration files). Note that additional data can be necessary to add initial conditions, boundary conditions, source terms (volume emissions, surface emissions) or loss terms (deposition velocities, scavenging). In the table, Gaussian represents any Gaussian model (`GaussianPlume`, `GaussianPuff`, `GaussianPlume_aer` or `GaussianPuff_aer`) as they all need the same data.

Table 2.1: Mandatory data for each models.

Model	Data necessary.
CastorTransport	Temperature, Pressure, Altitude, AirDensity, MeridionalWind ZonalWind VerticalDiffusion.
CastorChemistry	The same as CastorTransport and SpecificHumidity, LiquidWaterContent, Attenuation.
Polair3DTransport	MeridionalWind (for advection), ZonalWind (for advection), VerticalDiffusion (for diffusion), Horizontal_diffusion (if `Isotropic_diffusion` is set to no; this value is given in the main configuration file), Temperature (if `With_air_density` is set to yes or for microphysical scavenging model), Pressure (if `With_air_density` is set to yes or for microphysical scavenging model).
Polair3DChemistry	The same as Polair3DTransport and SpecificHumidity, Attenuation.
Polair3DChemistryAssimConc	The same as Polair3DChemistry.
Polair3DAerosol	The same as Polair3DChemistry and LiquidWaterContent, SnowHeight.
Gaussian	Temperature, Wind_angle, Wind (wind module), Inversion_height, Stability.

All data for Eulerian models are outputs of meteorological preprocessing programs:

- `meteo`, `Kz`, `attenuation` (and `Kz_TM` if you use Troen & Mahrt parameterization for vertical diffusion), for models of type "Polair3D" while using raw meteorological data from ECMWF.

- `MM5-meteo` (and `Kz_TM` if you use Troen & Mahrt parameterization for vertical diffusion) for models of type "Polair3D" while using raw meteorological data from model MM5;

- `MM5-meteo-castor` (and `Kz_TM` if you use Troen & Mahrt parameterization for vertical diffusion) for models of type "Castor" while using raw meteorological data from model MM5.

2.5.5 Models / Modules Compatibilities

Models of type "Polair3D" require two transport modules (one for advection and one for diffusion), while models of type "Castor" only require one transport module (which deals with advection and diffusion). This does not mean that a module could not be shared by both models (although there is no common module in current Polyphemus version).

Table 2.2 and Table 2.3 present a summary of the compatibility between models and modules. Note that Gaussian models are not included in these tables because they don't need any module.

Table 2.2: Compatibility between models and transport modules.

	AdvectionDST3	DiffusionROS2	TransportPPM
Polair3DTransport	X	X	
Polair3DChemistry	X	X	
Polair3DAerosol	X	X	
Polair3DChemistryAssimConc	X	X	
CastorTransport			X
CastorChemistry			X

Table 2.3: Compatibility between models and chemistry modules.

	Castor	RACM	RADM	SIREAM	Decay
Polair3DChemistry		X	X	X	X
Polair3DAerosol				X	X
Polair3DChemistryAssimConc		X	X		
CastorChemistry	X				

In Table 2.3, module names are shortened to be displayed on one line: `Castor` is actually `ChemistryCastor`, `RACM` is `ChemistryRACM`, `RADM` is `ChemistryRADM`, `SIREAM` is `ChemistryRACM-SIREAM`.

As for drivers, BaseDriver is the simplest and the most used of them. The other drivers available are:

- `StationaryDriver`: for local scale Eulerian simulations.
- `PlumeDriver`: for Gaussian plume model (with or without aerosol species).
- `PuffDriver`: for Gaussian puff model (with or without aerosol species).
- `OptimalInterpolationDriver`: for data assimilation (optimal interpolation), to be associated with `Polair3DAssimConc` model.

2.5.6 Checking Results

It is highly recommended to check the fields generated by Polyphemus programs: meteorological fields, deposition velocities, output concentrations, ...

First you can check the size of the binary files. The results are saved as floating point numbers with single precision. This means that most results file must be of size $4 \times N_t \times N_z \times N_y \times N_x$ bytes where N_x and N_y are the space steps along x and y directions respectively, N_z is the number of vertical levels of the field and N_t is the number of time steps. Note that, N_t is not the number of time steps of the simulation but the number of time steps *for which concentrations are saved.*

Second you should check that the fields have reasonable values using the programs from directory `utils`, mainly `get_info_float` (see Section 2.4.1). The command line to use `get_info_float` is:

```
get_info_float results/O3.bin
```

And the output looks like:

```
Minimum: 0.0563521
Maximum: 169.219
Mean:  91.3722
```

2.5.7 Important Notice

As for now, *under Linux*, `Talos` cannot read text files with Windows end-of-lines. In particular, if you send a configuration file through FTP or transfer it on a USB flash disk, chances are the coding system will be Windows and Talos won't be able to read the configuration.

In that case, to solve the problem if needed, simply open the file with `emacs`[†2].

If in the *mode line* (line at the bottom of the buffer) appears `(DOS)`, the coding system is incorrect. To modify it, type:

```
C-X <Ret> f <Ret>
```

Actually the last `<Ret>` sets the coding system to its default value, which is UNIX encoding.

[†2] `http://www.gnu.org/software/emacs/`

Chapter 3

Preprocessing

This chapter introduces all preprocessing programs. It details the input files (data files and configuration files) of every program, and it describes their output files. In Section 3.2, configurations and features shared by almost all programs are explained.

3.1 Remark

In the descriptions of preprocessing programs, there are references to functions like `ComputePressure`, `ComputeAttenuation_LWC`, etc. These functions are part of AtmoData and are described in AtmoData scientific documentation [Njomgang et al., 2005].

3.2 Introduction

3.2.1 Running Preprocessing Programs

Most preprocessing programs:

- accept one or two configuration files as arguments;
- process data day per day (one call to a program processes a single day);
- *append* their results at the end of binary files (if they already exist) or create them. Note that they cannot create the directory so you have to make sure it exists before launching a preprocessing program.

For instance, program `meteo` processes meteorological data over one day. To generate data from day 2001-05-19 to day 2001-05-21, one should launch:

```
./meteo ../general.cfg meteo.cfg 20010519
./meteo ../general.cfg meteo.cfg 20010520
./meteo ../general.cfg meteo.cfg 20010521
```

Another option is to use the script `call_dates` (see Section 2.4.4). In that case, to generate data from day 2005-05-19 to day 2005-05-21, one should launch:

```
meteo> ../utils/call_dates meteo ../general.cfg meteo.cfg 20050519 20050521
```

or

```
meteo> ../utils/call_dates meteo ../general.cfg meteo.cfg 20050519 3
```

Remember that *the results are appended at the end of the output files if they already exist.* If you decide to recompute your fields from the first day, you have to *first remove* old output binary files.

In order to know what are the arguments of a program, you may launch it without arguments. For instance:

```
emissions> ./emissions

Usage:
  ./emissions [main configuration file] [secondary configuration file] [date]
  ./emissions [main configuration file] [date]
  ./emissions [date]

Arguments:
  [main configuration file] (optional): main configuration file. Default: emissions.cfg
  [secondary configuration file] (optional): secondary configuration file.
  [date]: date in format YYYYMMDD.
```

3.2.2 Configuration

Almost all programs require the description of the domain over which computations should be performed. Since this configuration is shared by many programs, it is put in a common configuration file called `general.cfg`. An example of such a file is `Polyphemus/preprocessing/general.cfg`, whose content is quoted below:

```
[general]

Home: /u/cergrene/0/bordas
Directory_computed_fields: <Home>/B/data
Directory_ground_data: <Directory_computed_fields>/ground
Programs: <Home>/codes/Polyphemus-HEAD


[domain]

Date: 20010102
t-min = 0.0     Delta_t = 3.0   Nt = 9
x_min = -10.0   Delta_x = 0.5   Nx = 65
y_min = 40.5    Delta_y = 0.5   Ny = 33
Nz = 5
Vertical_levels: <Programs>/levels.dat
```

Entries in section `[general]` are markups provided for convenience. See Section 2.3.3 for further explanations.

The section `[domain]` contains the domain (in space and time) description.

[domain]	
`Date`	The date at which the simulation (of the chemistry-transport model) is starting. It is also the date at which meteorological data (processed by Polyphemus – output from programs `meteo` or `MM5-meteo`) starts. As a consequence, any program that needs to read this meteorological data refers to this date. The date must be in a format described in Section 2.2.7.
`t_min`	Hours at which the simulation is starting.
`Delta_t`	Time step in hour of *output meteorological data* processed by Polyphemus.
`Nt`	Number (integer) of meteorological steps per day.
`x_min`	Abscissa of the center of the lower-left cell. It is usually in longitude (degrees).
`Delta_x`	Step length along x, usually in degrees (longitude).
`Nx`	Number of cells along x (integer).
`y_min`	Ordinate of the center of the lower-left cell. It is usually in latitude (degrees).
`Delta_y`	Step length along y, usually in degrees (latitude).
`Ny`	Number of cells along y (integer).
`Nz`	Number of vertical levels (integer).
`Vertical_levels`	Path to the file that defines vertical levels interfaces in m.

3.2.3 Data Files

Polyphemus reads ECMWF Grib files, MM5 files, NetCDF files (for Mozart 2), text files and binary files. All files generated by Polyphemus are text files or binary files.

Unless specified otherwise, all binary files store single-precision floating-point numbers. They do not contain any header. Each binary file only stores the values of a single field. Four-dimensional fields are stored this way:

```
Loop on time t
   Loop on z
      Loop on y
         Loop on x
```

Let this storage be symbolized by $\{t, z, y, x\}$. Dimensions t, z, y and x always appear in this order. For instance, three-dimensional fields may be stored in formats $\{z, y, x\}$ or $\{t, y, x\}$, $\{t, z, x\}$ or $\{t, z, y\}$.

3.3 Ground Data

Computing ground data is the first step of a preprocessing as they are necessary to process meteorological fields. All programs related to ground-data generation are available in `Polyphemus/preprocessing/ground`.

The first step should be program `luc-usgs` or `luc-glcf` depending on what raw data you have. Land use data may come from the US Geological Survey (USGS) or from the Global Land Cover Facility (GLCF).

3.3.1 Land Use Cover – GLCF: `luc-glcf`

In order to prepare land use cover from GLCF, one should use program `luc-glcf`. It is recommended to download the global land use cover file at 1 km resolution provided in latitude–

longitude coordinates. At the time this documentation is written, the file is available[†1] at:

`ftp://ftp.glcf.umiacs.umd.edu/glcf/Global_Land_Cover/Global/gl-latlong-1km-landcover/gl-latlong-1km-landcover.bsq.gz` (single line, no white space – you may use `wget` to download it, or copy and paste the URL in your favorite browser).

You need to uncompress this file (e.g., `gunzip gl-latlong-1km-landcover.bsq.gz`).

Finally you have to fill the configuration file `luc-glcf.cfg`. Note that the default values in section `[GLCF]` are for file `gl-latlong-1km-landcover.bsq`: no need to change them if you downloaded this recommended file.

	`[paths]`
`Database_luc-glcf`	Directory where the raw data from GLCF can be found (directory where `gl-latlong-1km-landcover.bsq` lies).
`LUC_in`	Name of the file containing raw data (i.e., `gl-latlong-1km-landcover.bsq` or its new name if you renamed it).
`Directory_luc-glcf`	Output directory.
`LUC_out`	Output filename. The default filename `LUC-glcf.bin` is recommended for clarity.
	`[GLCF]`
`Step`	Space step in degrees in GLCF input file.
`x_min`	Minimum longitude in the input file (degrees).
`y_min`	Minimum latitude in the input file (degrees).
`Nx`	Number of cells along longitude in the input file.
`Ny`	Number of cells along latitude in the input file.
`Nc`	Number of land use categories.

The output land-cover file is in format $\{c, y, x\}$ where c stands for (land use) category.

To launch `luc-glcf`, just type:

```
./luc-glcf ../general.cfg luc-glcf.cfg
```

3.3.2 Land Use Cover – USGS: `luc-usgs`

For a simulation over Europe, program `luc-usgs` requires two files found at url `http://edcsns17.cr.usgs.gov/glcc/`:

- USGS Land Use/Land Cover Scheme for Eurasia in Lambert Azimuthal Equal Area Projection (optimized for Europe) available at `http://edcftp.cr.usgs.gov/pub/data/glcc/ea/lamberte/eausgs2_0le.img.gz` in compressed format.
- USGS Land Use/Land Cover Scheme for Africa in Lambert Azimuthal Equal Area Projection available at `http://edcftp.cr.usgs.gov/pub/data/glcc/af/lambert/afusgs2_0l.img.gz` in compressed format.

The configuration file `luc-usgs.cfg` requires:

[†1] In case the file has been moved, try to find it from `http://glcf.umiacs.umd.edu/data/landcover/`, or even from GLCF homepage `http://glcf.umiacs.umd.edu/index.shtml`.

	[paths]
Database_luc-usgs	Directory where the raw data from USGS can be found.
LUC_in_ea	Input file containing raw data for Eurasia.
LUC_in_af	Input file containing raw data for Africa.
Directory_luc-usgs	Output directory.
LUC_out	Output file name.The default filename LUC-usgs.bin is recommended for clarity.
	[USGS]
Step	Space step in meters.
lon_origin_ea	Longitude of the center of lower-right cell for Eurasia.
lat_origin_ea	Latitude of the center of the lower-right cell for Eurasia.
lon_origin_af	Longitude of the center of the lower-right cell for Africa.
lat_origin_af	Latitude of the center of the lower-right cell for Eurasia.
lon_upper_left_ea	Longitude of the center of the upper-left cell for Eurasia.
lat_upper_left_ea	Latitude of the center of the upper-left cell for Eurasia.
lon_upper_left_af	Longitude of the center of the upper-left cell for Africa.
lat_upper_left_af	Latitude of the center of the upper-left cell for Africa.
Nx_ea	Number of cells along longitude in the input file for Eurasia.
Nx_af	Number of cells along longitude in the input file for Africa.
Ny_ea	Number of cells along latitude in the input file for Eurasia.
Ny_af	Number of cells along latitude in the input file for Africa.
Nc	Number of land categories.
Sea_index	Index of the sea in land categories (Remember that indices start at 0).

The output land-cover file is in format $\{c, y, x\}$ where c stands for (land use) category.

To launch `luc-usgs`, just type:

```
./luc-usgs ../general.cfg luc-usgs.cfg
```

3.3.3 Conversions: `luc-convert`

The output of `luc-glcf` or `luc-usgs` are land use cover described with GLCF or USGS categories. It is often useful to convert these descriptions to another set of land use categories. This means, for example, summing up the contributions of sparsely vegetated and bare ground tundra (USGS categories #19 and #22) to estimate the proportion of barren land in Wesely description (category #8). An input category may also be split into several output categories. In practice, one may want to convert in Wesely or Zhang land use cover using `luc-convert`. In particular it is necessary to convert land data from USGS or GLCF to Zhang categories before computing deposition velocities with program `dep` (see Section 3.5.1).

In addition to the domain definition (Section 3.2.2), below is the information required in the configuration file (or configuration files) for `luc-convert`:

	[paths]
Database_luc-convert	Directory where the input file (input land use categories) is located.
File_in	Input file name (in Database_luc-convert).
Directory_luc-convert	Directory where the output file (output land use categories) should be stored.

File_out	Output file name (in Directory_luc-convert).
	[dimensions]
Nc_in	Number of land categories in the input format.
Nc_out	Number of land categories in the output format.
	[coefficients]
Correspondence matrix between input land categories and output land categories. Each line corresponds to an input category. Each line contains: the index of the category (or any number: this first column is not read) and the distribution of the input category in all output categories (columns). The distribution is a set of numbers in $[0, 1]$ whose sum should be 1.	

Several configuration files are provided to convert GLCF or USGS categories to Wesely or Zhang categories: glcf_to_wesely.cfg, glcf_to_zhang.cfg, usgs_to_wesely.cfg and usgs_to_zhang.cfg.

The output land-cover file is in format $\{c, y, x\}$ where c stands for (land use) category.

The conversion can be launched with:

```
./luc-convert ../general.cfg usgs_to_wesely.cfg
```

3.3.4 Roughness: roughness

After land use cover has been computed, roughness data can be estimated, using program roughness.

	[domain]
Nx	Number of grid points along longitude.
Ny	Number of grid points along latitude.
	[paths]
LUC_file	File where the land use cover data are stored (e.g., computed using luc-glcf or luc-usgs).
Directory_roughness	Directory where the output file will be stored.
Roughness_out	Output file name.
	[data]
Roughness_data_file	Path to the file giving the roughness of land categories. This file should be a text file with three columns: the land category index (starting at 0), the roughness height (in m) and the category name. Two examples are provided: roughness-glcf.dat and roughness-usgs.dat

The program may be launched with:

```
./roughness ../general.cfg roughness.cfg
```

Section [domain] is in general.cfg and the other sections are read in roughness.cfg.

3.4 Meteorological Fields

3.4.1 Program `meteo`

Program `Polyphemus/preprocessing/meteo/meteo` reads ECMWF Grib files and generates meteorological fields required by chemistry-transport models. Most fields are interpolated from ECMWF grid to a regular grid (latitude/longitude in the horizontal, altitudes in meters in the vertical). It is assumed that ECMWF input data are stored in daily Grib files.

Note that `meteo` needs as input data the land use cover which can be built using programs in `preprocessing/ground`.

The reference configuration files for `meteo` is `Polyphemus/preprocessing/meteo/meteo.cfg` together with `Polyphemus/preprocessing/general.cfg`. In addition to the domain definition, below are options of `meteo`:

	`[paths]`
`Database_meteo`	Directory in which ECMWF input files may be found. It is assumed that ECMWF file names are in format `ECMWF-YYYYMMDD` where `YYYY` is the year, `MM` the month and `DD` the day. If program `meteo` is launched for a day D, ECMWF data files for days D-1 and D must be available. Data for day D-1 are needed to process cumulated data (e.g., solar radiation).
`LUC_file`	Path to the binary file that describes land use cover over the *output* grid (described in section `[domain]`). This file must be in format $\{l, y, x\}$ (l is the land category) and it must contain proportions (in $[0, 1]$) of each land category in every grid cell.
`Sea_index`	Index of sea in land categories (recall that indices start at 0).
`Roughness_file`	Path to the binary file that describes roughness heights (in meters) in output grid cells. Its format is $\{y, x\}$. It is needed only if option `Flux_diagnosed` is activated.
`Roughness_in`	Path to the binary file that describes roughness heights (in meters) in ECMWF grid cells. Its format is $\{y, x\}$. It is needed only if option `Richardson_with_roughness` is activated.
`Directory_meteo`	Directory where output meteorological files are stored.
`Directory_Kz_TM`	Directory where the vertical diffusion using Troen and Mahrt parameterization is stored (output of `Kz_TM`).
	`[ECMWF]`
`t_min`	First hour stored in every ECMWF file.
`Delta_t`	Time step (in hour) of data stored in every ECMWF file.
`Nt`	Number of time steps stored in every ECMWF file.
`x_min`	Longitude in degrees of the center of the lower-left cell in ECMWF grid.
`Delta_x`	Step length (in degrees) along longitude of ECMWF grid.
`Nx`	Number of cells along longitude (integer) in ECMWF grid.
`y_min`	Latitude in degrees of the center of the lower-left cell in ECMWF grid.
`Delta_y`	Step length (in degrees) along latitude of ECMWF grid.
`Ny`	Number of cells along latitude (integer) in ECMWF grid.
`Nz`	Number of vertical layers (integer) in ECMWF grid.

	[meteo]
Richardson_with_roughness	Should the surface Richardson number be computed taking into account roughness height?
	[accumulated_data]
Accumulated_time	For data storing values cumulated in time (e.g., solar radiation), length number of time steps over which data is cumulated.
Accumulated_index	Start index of the first complete cycle of cumulated data. Data is then cumulated from t_min plus Accumulated_index times Delta_t.

The program basically reads data in the ECMWF Grib file and interpolates it in time and space to Polyphemus grid. ECMWF data is described in `meteo.cfg` and Polyphemus grid is described in `general.cfg`. For the sake of simplicity, it is recommended to work with ECMWF files containing data for one day: all Polyphemus programs work on a daily basis. Program `meteo` should be called for each day (preferably from 0h to 24h), that is, for each available ECMWF file (except the first one – see below). If ECMWF files are not provided on a daily basis, it is recommended to contact the Polyphemus team at `polyphemus@cerea.enpc.fr`.

In order to process the ECMWF file for a given day, the ECMWF file for the previous day must be available. Indeed, ECMWF files contain data that is accumulated over several time steps (like rain), and values from previous steps (including from the previous day) must be subtracted to get the actual value of the field.

Here is the list of input data needed in ECMWF files (with their Grib code): surface temperature (167), skin temperature (235), surface pressure (152), temperature (130), specific humidity (133), liquid water content (246), medium cloudiness (187), high cloudiness (188), meridional wind (132), zonal wind (131), zonal friction velocity (180), meridional friction velocity (181), solar radiation (169), boundary layer height (159), soil water content (39), sensible heat (146), evaporation (182).

The list of output variables is: pressure, surface pressure, temperature, surface temperature, skin temperature, Richardson number, surface Richardson number, specific humidity, liquid water content, solar radiation, photosynthetically active radiations (direct beam, diffuse and total), zonal wind, meridional wind, wind module, wind friction module, boundary layer height, soil water content, evaporation, sensible heat and first-level wind module.

Inside `meteo`, ECMWF variables are read and decumulated (in time) if necessary. Pressures at ECMWF levels are computed with `ComputePressure` and altitudes are computed with `ComputeInterfHeight` and `ComputeMiddleHeight`. Richardson number is then estimated with `ComputeRichardson`. All input fields are then interpolated on the vertical. Finally photosynthetically active radiation are estimated, based on solar radiation and zenith angle (`ZenithAngle`).

To get the complete set of input meteorological data for a transport model, one should then launch `attenuation`, `Kz` and maybe `Kz_TM`.

3.4.2 Program `attenuation`

Program `Polyphemus/preprocessing/attenuation` should be launched after program `meteo`. It computes cloud attenuation for photolysis rates. It also computes cloud related data, such as cloud height. Even for passive simulations this program should be launched.

The reference configuration files for `attenuation` is `Polyphemus/preprocessing/meteo/meteo.cfg` together with `Polyphemus/preprocessing/general.cfg`. In addition to the domain definition and to the entries of `meteo.cfg` introduced in Section 3.4.1, below are options for `attenuation`:

	`[paths]`
`Directory_attenuation`	Directory where the output of program `attenuation` is stored.
	`[attenuation]`
`Type`	Parameterization to be used to compute cloud attenuation. Put `1` to use `RADM` parameterization or put `2` to use `ESQUIF` parameterization.
	`[clouds]`
`Min_height`	Minimum cloud basis height in m.

Just like in program `meteo`, ECMWF data is read and interpolated. Then the relative humidity and the critical relative humidity are computed respectively with `ComputeRelativeHumidity` and `ComputeCriticalRelativeHumidity`. The cloud fraction is computed with `ComputeCloudFraction`. For it the cloudiness and cloud height are diagnosed using `ComputeCloudiness` and `ComputeCloudHeight`. Finally attenuation coefficients are computed with `ComputeAttenuation_LWC` (RADM parameterization) or `ComputeAttenuation_ESQUIF` (ESQUIF parameterization).

Output files are:

- the rain intensity (`Rain.bin`) in $\mathrm{mm\,h^{-1}}$,
- the convective rain intensity (`ConvectiveRain.bin`) in $\mathrm{mm\,h^{-1}}$,
- the 3D cloud attenuation coefficient (in $[0, 2]$),
- the cloud height in m.

3.4.3 Program `Kz`

Program `Kz` computes the vertical diffusion coefficients (needed in almost all applications) using Louis parameterization [Louis, 1979]. It should be launched after `attenuation`.

The reference configuration files for `Kz` is `Polyphemus/preprocessing/meteo/meteo.cfg` together with `Polyphemus/preprocessing/general.cfg`. In addition to the domain definition and to the entries of `meteo.cfg` introduced in Section 3.4.1 and 3.4.2, below are options for `Kz`:

	`[paths]`
`File_Kz`	Name of the file where the vertical diffusion coefficients (output) are stored.
	`[Kz]`
`Min`	Lower threshold for vertical diffusion in $\mathrm{m^2\,s^{-1}}$.
`Max`	Higher threshold for vertical diffusion in $\mathrm{m^2\,s^{-1}}$.
`Apply_vert`	If set to `no`, the lower threshold is applied only at the top of the first layer, otherwise it is applied to all levels.

This programs mainly computes the vertical diffusion coefficients with a call to `ComputeLouisKz`.

Simple corrections are also performed to take into account convective conditions.

The output is a 3D time-dependent field (format $\{t, z, y, x\}$) of vertical diffusion coefficients (in $m^2\,s^{-1}$). Along the vertical, the coefficients are defined on the interfaces. So the size of the field (for each day) is $Nt \times (Nz+1) \times Ny \times Nx$. It is stored in the path given by entry `File_Kz`.

3.4.4 Program `Kz_TM`

Program `Kz_TM` "overwrites", in the boundary layer height, the vertical diffusion coefficients computed with Louis parameterization, with coefficients computed according to Troen & Mahrt parameterization [Troen and Mahrt, 1986]. It should be launched either after `Kz` or after `MM5-meteo`.

The reference configuration files for `Kz_TM` is `Polyphemus/preprocessing/meteo/meteo.cfg` or `Polyphemus/preprocessing/meteo/MM5-meteo.cfg` together with `Polyphemus/preprocessing/general.cfg`. In addition to the domain definition in `general.cfg`, below are the entries for `Kz_TM`:

	`[path]`
`LUC_file`	Path to the binary file that describes land use cover over the *output* grid (described in section `[domain]`). This file must be in format $\{l, y, x\}$ (l is the land category) and it must contain proportions (in $[0, 1]$) of each land category in every grid cell.
`Sea_index`	Index of sea in land categories (remember that indices start at 0).
`Roughness_file`	Path to the binary file that describes roughness heights (in meters) in output grid cells. Its format is $\{y, x\}$. It is needed only if option `Flux_diagnosed` is activated.
`Directory_meteo`	Directory where output meteorological files are stored.
`File_Kz`	Name of the file where the vertical diffusion coefficients as computed with the Louis parameterization are stored.
`Directory_Kz_TM`	Name of the directory where the vertical diffusion coefficients (output) are stored (the filename being `Kz_TM`).
	`[Kz]`
`Min`	Lower threshold for vertical diffusion in $m^2\,s^{-1}$.
`Max`	Higher threshold for vertical diffusion in $m^2\,s^{-1}$.
`Apply_vert`	If set to `no`, the lower threshold is applied only at the top of the first layer, otherwise it is applied to all levels.
`p`	Coefficient used in Troen and Mahrt parameterization (see Troen and Mahrt [1986]).
`C`	Coefficient used in Troen and Mahrt parameterization (see Troen and Mahrt [1986]).
`SBL`	Ratio between the surface layer and the atmospheric boundary layer (0.1 in Troen and Mahrt [1986]).
`Ric`	Critical Richardson number used to estimate the atmospheric boundary layer height (in case `BL_diag` is set to `2`).
`Fluxes_diagnosed`	Should the friction module, the evaporation and the sensible heat be diagnosed? If not, they are read in input data (which is recommended).

BL_diag	What kind of diagnosis is used to estimate the boundary layer height? Put 1 to use Troen and Mahrt diagnosis [Troen and Mahrt, 1986]; put 2 to rely on a critical Richardson number; and put 3 to use ECMWF (or MM5) boundary layer height (so, there is no diagnosis – this option is more robust and it is recommended).
TM_stable	The vertical diffusion as computed by Troen and Mahrt parameterization is applied only within the boundary layer. It is possible to further restrict its application: if TM_stable is set to no, the parameterization is not applied in stable conditions. In this case, the Troen and Mahrt parameterization is only applied in unstable boundary layer.

Several meteorological fields are computed with ComputePotentialTemperature, ComputeSaturationHumidity and ComputeSurfaceHumidity_diag. If fluxes are not diagnosed, the Monin-Obukhov length is computed with ComputeLMO. Then the boundary layer height may be diagnosed with ComputePBLH_TM (Troen & Mahrt parameterization) or ComputePBLH_Richardson (critical Richardson number). Finally the vertical diffusion coefficients are computed with ComputeTM_Kz.

The main output is a 3D time-dependent field (format $\{t, z, y, x\}$) of vertical diffusion coefficients (in $m^2\,s^{-1}$). Along the vertical, the coefficients are defined on the interfaces. So the size of the field (for each day) is $Nt \times (Nz + 1) \times Ny \times Nx$. It is stored in Kz_TM.bin in the directory given by entry Directory_Kz_TM. The surface relative humidity is saved in SurfaceRelativeHumidity.bin. Depending on the options, additional fields may be saved, such as the Monin-Obukhov length in file LMO.bin.

3.4.5 Program MM5-meteo

Program Polyphemus/preprocessing/meteo/MM5-meteo processes MM5 data and generates meteorological fields required by chemistry-transport models. Most fields are interpolated from MM5 grid to a regular grid (latitude/longitude in the horizontal, altitudes in meters in the vertical).

Note that MM5-meteo needs as input data the land use cover which can be built using programs in preprocessing/ground.

Note for ECMWF users: program MM5-meteo is equivalent to what is performed by meteo, attenuation and Kz successively. As for ECMWF files, Kz_TM can be used afterwards.

The configuration file MM5-meteo.cfg contains several options:

[paths]	
Database_MM5_meteo	Directory in which MM5 input files may be found. If &D appears in the file name, it is replaced by MM5-YYYY-MM-DD where YYYY is the year, MM the month and DD the day.
LUC_file	Path to the binary file that describes land use cover over the *output* grid (described in section [domain]). This file must be in format $\{l, y, x\}$ (l is the land category) and it must contain proportions (in $[0, 1]$) of each land category in every grid cell.
Sea_index	Index of sea in land categories (remember that indices start at 0).
Roughness_file	Path to the binary file that describes roughness heights (in meters) in output grid cells. Its format is $\{y, x\}$. It is needed only if option Flux_diagnosed is activated.

`Directory_meteo`	Directory where output meteorological files are stored.
`Directory_attenuation`	Directory where the output of program `attenuation` is stored.
`File_Kz`	Name of the file where the vertical diffusion coefficients (computed according to Louis parameterization) are stored.
	`[MM5]`
`t_min`	First hour stored in every MM5 file.
`Delta_t`	Time step (in hour) of data stored in every MM5 file.
`Nt`	Number of time steps stored in every MM5 file.
`x_min`	Index in MM5 coordinates of the center of the lower-left cell in MM5 grid. This is most likely `0.5`.
`Delta_x`	Index (MM5 coordinates) increase along longitude of MM5 grid. This is most likely `1`.
`Nx`	Number of cells (or dot points) along longitude (integer) in MM5 grid.
`y_min`	Index in MM5 coordinates of the center of the lower-left cell in MM5 grid. This is most likely `0.5`.
`Delta_y`	Index (MM5 coordinates) increase along latitude of MM5 grid. This is most likely `1`.
`Ny`	Number of cells (or dot points) along latitude (integer) in MM5 grid.
`Nz`	Number of vertical layers (integer) in MM5 grid.
`projection_type`	Type of projection. `1` corresponds to Lambert conformal conic, `2` to Mercator and `3` to stereographic.
	`[accumulated_rain]`
`Prev_accumulated_rain`	Is the rain accumulated from the previous day?
	`[attenuation]`
`Type`	Parameterization to be used to compute cloud attenuation. Put `1` to use `RADM` parameterization or put `2` to use `ESQUIF` parameterization.
	`[clouds]`
`Min_height`	Minimum cloud basis height in m.
	`[Kz]`
`Min`	Lower threshold for vertical diffusion in $m^2\,s^{-1}$.
`Max`	Higher threshold for vertical diffusion in $m^2\,s^{-1}$.
`Apply_vert`	If set to `no`, the lower threshold is applied only at the top of the first layer, otherwise it is applied to all levels.

The program basically reads data in MM5 output file and interpolates it in time and space to Polyphemus grid. MM5 file is described in `MM5-meteo.cfg` and Polyphemus grid is described in `general.cfg`. Note that each time a field is loaded by `MM5-meteo`, all time steps are loaded in memory. Note that the fields are released from memory when unused, but you may still need a lot of memory for big MM5 output files.

The program first computes the altitude of MM5 layers, and converts the Polyphe-

mus grid coordinates (latitude/longitude) to MM5 grid coordinates (Lambert, Mercator or stereographic) for interpolations. Interpolations on the horizontal are performed in MM5 grid for efficiency. The pressure is computed based on MM5 fields. The winds are rotated: this gives meridional and zonal winds. The Richardson number is then computed (`ComputeRichardson`). The relative humidity and the critical relative humidity are computed respectively with `ComputeRelativeHumidity` and `ComputeCriticalRelativeHumidity`. The cloud fraction is computed with `ComputeCloudFraction`. For it the cloudiness and cloud height are diagnosed using `ComputeCloudiness` and `ComputeCloudHeight`. Finally attenuation coefficients are computed with `ComputeAttenuation_LWC` (RADM parameterization) or `ComputeAttenuation_ESQUIF` (ESQUIF parameterization). The vertical diffusion coefficients are computed with `ComputeLouisKz` [Louis, 1979]. Finally photosynthetically active radiation are estimated, based on solar radiation and zenith angle (`ZenithAngle`).

Among output files one may find:

- the pressure and the surface pressure in Pa,
- the temperature, the surface temperature and the skin temperature in K,
- the meridional and zonal winds (`MeridionalWind.bin` and `ZonalWind.bin`) in $\mathrm{m\,s^{-1}}$,
- the Richardson number and the surface Richardson number,
- the boundary layer height in m,
- the vertical diffusion coefficients (time-dependent 3D field, defined on layer interfaces on the vertical, `Kz_Louis.bin`) in $\mathrm{m^2\,s^{-1}}$,
- the specific humidity in $\mathrm{kg\,kg^{-1}}$,
- the liquid water content in $\mathrm{kg\,kg^{-1}}$,
- the cloud attenuation coefficients (3D field, `Attenuation.bin`) in $[0, 2]$,
- the solar radiation intensity (`SolarRadiation.bin`) in $\mathrm{W\,m^{-2}}$,
- the rain intensity (`Rain.bin`) in $\mathrm{mm\,h^{-1}}$,
- the convective rain intensity (`ConvectiveRain.bin`) in $\mathrm{mm\,h^{-1}}$,
- the cloud height in m.

3.4.6 Program `MM5-meteo-castor`

Program `MM5-meteo-castor` processes MM5 data and generates meteorological fields required by chemistry-transport model Castor.

[paths]	
`Database_MM5_meteo`	Directory in which MM5 input files may be found. If `&D` appears in the file name, it is replaced by `YYYY-MM-DD` where `YYYY` is the year, `MM` the month and `DD` the day.
`Roughness_file`	Path to the binary file that describes roughness heights (in meters) per month in output grid cells.
`Hybrid_coefficients`	File containing the parameters alpha and beta used to compute the pressure at various levels and the altitudes.

`Directory_meteo`	Directory where output meteorological files are stored.
	`[MM5]`
`t_min`	First hour stored in every MM5 file.
`Delta_t`	Time step (in hour) of data stored in every MM5 file.
`Nt`	Number of time steps stored in every MM5 file.
`x_min`	Index in MM5 coordinates of the center of the lower-left cell in MM5 grid. This is most likely `0.5`.
`Delta_x`	Index (MM5 coordinates) increase along longitude of MM5 grid. This is most likely `1`.
`Nx`	Number of cells (or dot points) along longitude (integer) in MM5 grid.
`y_min`	Index in MM5 coordinates of the center of the lower-left cell in MM5 grid. This is most likely `0.5`.
`Delta_y`	Index (MM5 coordinates) increase along latitude of MM5 grid. This is most likely `1`.
`Ny`	Number of cells (or dot points) along latitude (integer) in MM5 grid.
`Nz`	Number of vertical layers (integer) in MM5 grid.
`projection_type`	Type of projection. `1` corresponds to Lambert conformal conic, `2` to Mercator and `3` to stereographic.
`Horizontal_interpolation`	Type of horizontal interpolation used. `MM5` corresponds to MM5 coordinates and `latlon` to latitude/longitude coordinates.
`Dot_coordinates`	File containing coordinates of dot points. Used if `Horizontal_interpolation` is set to `latlon`.
	`[meteo]`
`Relative_humidity_threshold`	Minimum relative humidity above which cloud are formed.
`Low_cloud_top_max`	Low clouds maximum height (in m).
	`Kz]`
`Min_dry`	Minimum value of Kz in PBLH for dry conditions (in $m\,s^{-2}$).
`Min_wet`	Minimum value of Kz in PBLH for cloudy conditions (in $m\,s^{-2}$).
`Min_above_PBLH`	Minimum value of Kz above PBLH (in $m\,s^{-2}$).
`Max`	Maximum value for Kz (in $m\,s^{-2}$).

Among output files one may find:

- the altitude in meters,
- the air density (`AirDensity.bin`)
- the pressure in Pa (`Pressure.bin`),
- the temperature and temperature at 2 m in K (`Temperature.bin` and `Temperature_2m.bin`),
- the meridional wind , zonal wind, convective velocity and wind module at 10 m (`MeridionalWind.bin`, `ZonalWind.bin`, `ConvectiveVelocity.bin` and `WindModule_10m.bin`) in $m\,s^{-1}$,

- the boundary layer height in m (`PBLH.bin`),
- the vertical diffusion coefficients using Troen and Mahrt parameterization (`Kz.bin`) in $m^2\,s^{-1}$,
- the specific humidity in $kg\,kg^{-1}$ (`SpecificHumidity.bin`),
- the surface relative humidity (`SurfaceRelativeHumidity.bin`,
- the liquid water content in $kg\,kg^{-1}$ (`LiquidWaterContent.bin`),
- the cloud attenuation coefficients (`Attenuation.bin`)
- the soil moisture (`SoilMoisture.bin`),
- the aerodynamic resistance (`AerodynamicResistance.bin`),
- the friction velocity in $m\,s^{-1}$ (`FrictionModule.bin`),

3.5 Deposition Velocities

Deposition velocities are generated on the basis of meteorological fields and land data. The programs must be launched after meteorological and ground preprocessing.

The computation of deposition velocities for Gaussian models is presented in Section 3.9.2.

3.5.1 Program `dep`

The program `dep` computes deposition velocities according to Wesely [1989] or Zhang et al. [2003].

In addition to `general.cfg`, the program reads the configuration in `dep.cfg`. In this file, paths to several files generated by programs `meteo` or `MM5-meteo` are given.

[paths]	
`SurfaceTemperature`	File where surface temperature is stored.
`SurfaceRichardson`	File where surface Richardson number is stored.
`SolarRadiation`	File where solar radiation is stored.
`WindModule`	File where wind module is stored.
`PAR`	File where photosynthetically active radiation is stored.
`PARdiff`	File where the diffuse part of the photosynthetically active radiation is stored.
`PARdir`	File where the direct beam part of photosynthetically active radiation is stored.
`SpecificHumidity`	File where (3D) specific humidity is stored.
`SurfacePressure`	File where surface pressure is stored.
`FrictionVelocity`	File where friction velocity is stored.
`CanopyWetness`	File where canopy wetness is stored.
`Rain`	File where rain is stored.
`RoughnessHeight`	File where roughness height is stored.
`Type`	Configuration file that describes land use cover (see below for details about this file).

`Data`	File containing the data for species. This file should contain: the species name, the molecular weight ($g\,mol^{-1}$), Henry constant, diffusivity, reactivity, alpha [Zhang et al., 2003], beta [Zhang et al., 2003], Rm. An example for RADM/RACM is available in `preprocessing/dep/input/species_data.txt`.
`Directory_dep`	Directory where the output files are stored.
	`[Species]`
`Ns`	Number of species for which data are provided. This should be the number of columns in `preprocessing/dep/input/species_data.txt`.
	`[Options]`
`CellRoughness`	If this option is set to `yes`, the roughness height used in calculations only depends on the model cell (and not on the land use category). In this case, it uses the data file whose path is given in entry `RoughnessHeight` (section `[paths]`). If the options is set to `no` (recommended), the roughness height depends on the land use category (see entry `Type`).
`Ra`	Parameterization used to compute the aerodynamic resistance. You can choose between `fh` (heat flux), `fm` (momentum flux) or `diag` (diagnostic).
`Rb`	Parameterization used to compute the quasi-laminar sublayer resistance. You can choose between `friction` and `diag`.
`Rc`	Parameterization used to compute the canopy resistance (Zhang et al. [2003] or Wesely [1989]).
`Save_resistance`	Should Ra, Rb and Rc be saved? This may take a lot of storage space: put `no` if you do not work on the deposition parameterizations.

Entry `Type` is the path to a configuration file whose entries should be:

`File`	Path to the file describing the land use cover. The number of categories in the file is deduced from its size, but it must be consistent with the data provided in the following entries (`Midsummer`, etc.)
`Midsummer`	Data file for midsummer (see below for details).
`Autumn`	Data file for autumn (see below for details).
`Late_autumn`	Data file for late autumn (see below for details).
`Snow`	Data file for snow (see below for details).
`Spring`	Data file for spring (see below for details).

The data files mentioned above for the five "seasons" must contain a column for each land use category with 22 parameters in each column. You may modify these files or create new files only if you are well aware of deposition parameterizations. With Polyphemus, a set of 5 files is provided for convenience, and any beginner should use them. They are suited for land use categories as defined in Zhang et al. [2002].

A key step is therefore to generate a land use description with these categories (referred as Zhang categories). The recommended program to generate this file is `luc-convert` which is described in Section 3.3.3. You should use this program to convert GLCF or USGS land cover

to Zhang categories.

The program may be launched this way:

```
./dep ../general.cfg dep.cfg 20040809
```

3.5.2 Program `dep-emberson`

The program `dep-emberson` is used to compute deposition velocities for Castor model, using Emberson parameterization.

	`[paths]`
`Altitude`	File where altitude is stored.
`SurfaceTemperature`	File where surface temperature is stored.
`SurfaceRelativeHumidity`	File where surface relative humidity is stored.
`FrictionVelocity`	File where the friction velocity is stored.
`Attenuation`	File where the attenuation is stored.
`AerodynamicResistance`	File where the aerodynamic resistance is stored.
`LUC_file`	File containing the land use cover.
`Nc`	Number of land use cover categories.
`Nveg`	Number of vegetation classes.
`Land_data`	File containing land data in Chimere format.
`Species_data`	File containing the data for species (molecular weight, Henry constant, reactivity).
`Directory_dep`	Directory where the output files are stored.
	`[Species]`
`Ns`	Number of species for which data are provided.

The program must be launched with:

```
./dep-emberson ../general.cfg dep-emberson.cfg 20040809
```

3.6 Emissions

Emissions are generated on the basis of land data (anthropogenic emissions) and meteorological fields (biogenic emissions). The programs must be launched after meteorological and ground preprocessing.

For Gaussian models, a preprocessing step may also be required in case line emissions are included (see Section 3.9.1).

3.6.1 Mapping Two Vertical Distributions: `distribution`

Program `distribution` may be used to define the distribution of emissions along the vertical. It reads the vertical distribution of emissions in some input grid and maps this distribution on an output vertical grid. Thus it generates a file with the vertical distribution of emissions in the output grid. It is based on AtmoData function `ComputeVerticalDistribution`.

Running this program is not compulsory. Even if the vertical distribution of emissions is required to compute anthropogenic emissions (program `emissions`), the vertical distribution can be generated by other means (including "by hand").

	`[domain]`
`Nz`	Number of output vertical levels.
`Vertical_levels`	Path to the text file that stores the altitudes (in m) of output level interfaces (hence `Nz+1` values are read).
	`[EMEP]`
`Nz_in`	Number of input vertical levels.
`Vertical_levels`	Path to the text file that stores the altitudes (in m) of input level interfaces (hence `Nz_in+1` values are read).
`Vertical_distribution`	Path to the file with the input vertical distribution of emissions. This file should contain one line per emission sector. Each line contains the percentage of emissions at ground level (first column) and the percentage of emissions in each vertical level (`Nz_in` following columns).
`Polair_vertical_distribution`	Path to the output file where the output vertical distribution of emissions should be stored. The format is the same as in file `Vertical_distribution`.
`Nsectors`	Number of activity sectors.

3.6.2 Anthropogenic Emissions (EMEP): `emissions`

Program `emissions` processes an EMEP emission inventory and generates (anthropogenic) surface and volume emissions needed by Polair3D.

First you must download Expert emissions inventories from `http://webdab.emep.int/`. Download emissions for CO, NH3, NNMVOC, NOx, SOx, PM2.5 and PMcoarse and make sure to have a file for each species called `CO.dat`, `NH3.dat`, `NMVOC.dat`, `NOX.dat`, `SOX.dat`, `PM2.5.dat` and `PMcoarse.dat`.

Download files with the following options:

- for all countries;
- for the year of your choice (up to 2004);
- for all activity sectors (SNAP) or, even better, without the eleventh EMEP sector whose emissions are better estimated with program `bio` (Section 3.6.3);
- in format "Grid (50 km $\times$ 50 km), Semicolon-Separated";
- for one species.

In addition to the domain definition (Section 3.2.2), program `emissions` reads a configuration file such as `emissions.cfg`:

	`[paths]`
`Directory_surface_emissions`	Directory where the computed surface emissions are stored.
`Directory_volume_emissions`	Directory where the computed volume emissions are stored. This should be different from `Directory_surface_emissions` since files for surface emissions and volume emissions have the same names (species names).

	[EMEP]
Polair_vertical_distribution	File where the vertical distribution of emissions is stored. This file should contain one line per emission sector. Each line contains the percentage of emissions at ground level (first column) and the percentage of emissions in each vertical level (Nz following columns).
Input_directory	Directory containing EMEP emissions inventory.
Hourly_factors	File defining hourly factors (see below).
Weekdays_factors	File defining weekdays factors (see below).
Monthly_factors	File defining monthly factors (see below).
Time_zones	File defining the time zone for various countries.
Nx_emep	Number of cells along longitude (integer) in EMEP grid.
Ny_emep	Number of cells along latitude (integer) in EMEP grid.
Ncountries	Maximum number of countries covered by the inventory.
Species	Names of inventory species.
Nsectors	Number of activity sectors.
Urban_ratio	Emission ratio for urban areas (see below).
Forest_ratio	Emission ratio for forest (see below).
Other_ratio	Emission ratio for other areas (see below).
	[LUC]
File	Path to land use cover file.
x_min	Longitude in degrees of the center of the lower-left cell in LUC grid.
Delta_x	Step length (in degrees) along longitude of LUC grid.
Nx	Number of cells along longitude (integer) in LUC grid.
y_min	Latitude in degrees of the center of the lower-left cell in LUC grid.
Delta_y	Step length (in degrees) along latitude of LUC grid.
Ny	Number of cells along latitude (integer) in LUC grid.
	[Species]
N	Number of emitted species.
Aggregation	Aggregation matrix file (relations of the emitted species to the real chemical species).
Speciation_directory	Directory in which, for each inventory species XXX, a file XXX.dat contains the speciation to real chemical species as function of the emission sector (columns).
Deposition_factor_NH3	Part of emitted NH_3 which is deposited right away.

The program emissions reads EMEP emissions inventory, multiplies them by temporal factors and interpolates them on Polair3D grids. EMEP emissions are read with AtmoData function ReadEmep. The spatial interpolation is performed with EmepToLatLon.

Urban, forest and "other" ratios Ratios Urban_ratio, Forest_ratio and Other_ratio enable to distribute emissions of an EMEP cell according to the type of land (urban, forests and other categories). For instance, in an EMEP cell, emissions are distributed so that the ratio between total urban emissions and total emissions is Urban_ratio on top of the sum of

Urban_ratio, Forest_ratio and Other_ratio.

Temporal Factors EMEP emissions are provided as annual values. They are multiplied by temporal factors to estimate their time evolution (as function of month, week day and hour) in all emission sectors and in all countries.

Here are examples on how these factors should be provided:

- monthly_factors.dat gives the factors for each country index (CC), each activity sector (SNAPsector) and each month.

```
# Formate: CC SNAPsector  JAN    FEB    MAR    APR    MAY    JUN    JUL  ...
2  1  1.640  1.520  1.236  1.137  0.798  0.459  0.393 ..
```

- weekdays_factors.dat gives the factors for each country index (CC), each activity sector (SNAPsector) and each day of the week.

```
# Formate: CC SNAPsector  MON      TUE      WED      Thu      FRI      SAT      SUN
2  1  1.0159   1.0348   1.0399   1.0299   1.0298   0.9651   0.8846
```

- hourly_factors.dat gives the factor for each activity sector (SNAPsector) and each hour.

```
#  1   2   3   4   5   6   7   8   9  10  11  12  13  14  15  16  17  ...
1  1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 ...
```

3.6.3 Biogenic Emissions for Polair3D Models: bio

Program bio computes biogenic emissions on the basis of meteorological fields and land use cover.

In addition to the domain definition (Section 3.2.2), below is the information required in the configuration for bio (see example bio.cfg):

[paths]	
SurfaceTemperature	Binary file where the surface temperature is stored.
PAR	Binary file where the photosynthetically active radiation is stored.
LUC_file	Binary file where the land use cover is stored.
Land_data	Data file giving emission factors for isoprene, terpenes and NO_x for all land categories defined in LUC_file. In this file, each line (which is not empty or does not start with "#") provides data for one land use category. for such a line, the first 55 characters are discarded: you may put the category number and description for convenience. Then four columns are read with the biomass density ($g\,m^{-2}$), and the emission factors for isoprene, terpenes and NO_x (in this order). Two examples are provided with land_data_glcf.dat and land_data_usgs.dat, to be used in combination with land use cover generated by luc-glcf or luc-usgs respectively.
Directory_bio	Directory where output biogenic emissions are stored.

	[biogenic]
Delta_t	Time step (in hours) for the output biogenic emissions. For simulations with Polair3D, anthropogenic emissions and biogenic emissions must have the same time step (that is, usually one hour).
Rates	Should emission rates be saved? These rates are not needed by chemistry-transport models.
Terpenes	Names of the species included in terpenes emissions. For RACM Stockwell et al. [1997], put API and LIM.
Terpenes_ratios	Distribution of terpenes emissions among species (entry Terpenes).

Biogenic emissions are computed according to Simpson et al. [1999]. Meteorological data is first interpolated in time so that its time step is Delta_t (section [biogenic]). Emission rates are then computed using AtmoData function ComputeBiogenicRates and emissions using ComputeBiogenicEmissions.

3.6.4 Sea Salt Emissions: sea-salt

Program sea_salt computes the emissions of sea-salt aerosols. Its options and parameters are given in sea_salt.cfg.

	[paths]
Surface_wind_module_file	Binary where the wind module at surface is stored.
Directory_sea_salt	Directory where sea-salt emissions are stored.
	[sea_salt]
Threshold_radius	Radius above which Monahan parameterization is used (in µm).
Delta_t	Time step for sea-salt emissions computation.
	[LUC]
File	File containing land use cover.
Nb_luc	Number of land categories.
Sea_index	Index of sea in land categories (recall that indices start at 0).
	[PM]
Section_computed	Should diameter classes bounds be computed? Otherwise they are read in File_sections.
Diameter_min	Minimum diameter if diameter classes bounds are computed.
Diameter_max	Maximum diameter if diameter classes bounds are computed.
Nsections	Number of diameter classes.
File_sections	File containing the diameter classes bounds if they are not computed.

3.7 Initial Conditions: `ic`

Climatological concentrations from Mozart 2 [Horowitz et al., 2003] (Home page at `http://gctm.acd.ucar.edu/mozart/index.shtml`) are used to generate initial concentrations for photochemistry simulation with Polair3D. Program `ic` has been tested with Mozart 2 output files downloaded on NCAR data portal at `https://cdp.ucar.edu/`.

In addition to the domain definition (Section 3.2.2), below is the information required in the configuration for `ic` (see example `ic.cfg`):

	`[ic_input_domain]`
`Date_ic`	Date for which initial conditions are generated.
`Nt`	Number of time steps in Mozart 2 files.
`Delta_t`	Time step of Mozart 2 files (in hours).
`Nx`	Number of grid points along latitude in Mozart 2 files (integer).
`Ny`	Number of grid points along longitude in Mozart 2 files (integer).
`Nz`	Number of vertical levels in Mozart 2 files (integer).
`Database_ic`	Directory where the Mozart 2 files are available. Mozart 2 filenames are in form `h00xx.nc` where `xx` is computed by the program according to the date `Date_ic`.
	`[ic_files]`
`Species`	File providing correspondence between the name of species in Mozart 2 files and the name of species in simulation. In this file, the first column contains Mozart 2 species. After each Mozart 2 species name, the corresponding output species (e.g., RACM species) is put, if any. If Mozart 2 species gathers two output species, put the names of all output species followed by their proportion in Mozart 2 bulk species. For instance, the line `C4H10 HC5 0.4 HC8 0.6` splits Mozart 2 species `C4H10` into `HC5` (40%) and `HC8` (60%). Three examples are provided: `preprocessing/bc/species_v1.dat`, `preprocessing/bc/species_v2.dat` and `preprocessing/bc/species_v3.dat`.
`Molecular_weight`	File providing the molecular weights of output species.
`Directory_ic`	Directory where the output initial conditions must be stored.

The name of the Mozart 2 files must be in the form `h00xx.nc` where `xx` is computed as follows: $xx = 40 + \lfloor \frac{N_d+6}{10} \rfloor$ and where N_d is the number of days since the beginning of the year (0 for first January). In case your Mozart 2 files do not satisfy this format (this may happen if Mozart files are updated on the NCAR data portal), you may modify the code or contact Polyphemus team at `polyphemus@cerea.enpc.fr`.

3.8 Boundary Conditions

3.8.1 Boundary Conditions for Gaseous Species: `bc`

In addition to the domain definition (Section 3.2.2), below is the information required in the configuration for `bc` (see example `bc.cfg`):

	[bc_input_domain]
Nt	Number of time steps in Mozart 2 files.
Delta_t	Time step of Mozart 2 files (in hours).
Nx	Number of grid points along latitude in Mozart 2 files (integer).
Ny	Number of grid points along longitude in Mozart 2 files (integer).
Nz	Number of vertical levels in Mozart 2 files (integer).
	[bc_files]
Directory_bc	Directory where the output boundary conditions must be stored.
Species	File providing correspondence between the name of species in Mozart 2 files and the name of species in simulation. In this file, the first column contains Mozart 2 species. After each Mozart 2 species name, the corresponding output species (e.g., RACM species) is put, if any. If Mozart 2 species gathers two output species, put the names of all output species followed by their proportion in Mozart 2 bulk species. For instance, the line `C4H10 HC5 0.4 HC8 0.6` splits Mozart 2 species `C4H10` into `HC5` (40%) and `HC8` (60%). Three examples are provided: `preprocessing/bc/species_v1.dat`, `preprocessing/bc/species_v2.dat` and `preprocessing/bc/species_v3.dat`.
Molecular_weight	File providing the molecular weights of output species.

Program `bc` processes an entire Mozart 2 output file. If this file contains concentrations for 10 days, the program generates boundary conditions for 10 days.

The program must be launched with:

```
./bc bc.cfg ../general.cfg /net/libre/adjoint/mallet/mozart/h0067.nc
```

The last argument is the path to the Mozart 2 file. You have to select the file to use according to date as what is shown in Section 3.7.

The results are stored as `&f_&c.bin` where `&f` is replaced by the name of the species and `&c` by the direction associated with the boundary condition (x, y or z). For example, the concentrations in `O3_x.bin` are interpolated at both ends of the domain along x, for all grid points along y and z.

3.8.2 Boundary Conditions for Aerosol Species: `bc-gocart`

Boundary conditions for aerosol species are obtained using Gocart model[†2] thanks to the program `bc-gocart`.

Gocart format and conventions

Gocart model usually provides files with the following naming convention:

file name	signification
yyyymm.XX.vs.g	6-hourly concentrations in $\mathrm{g\,m^{-3}}$.
yyyymm.XX.vs.g.day	daily averaged concentrations in $\mathrm{g\,m^{-3}}$.
yyyymm.XX.vs.g.avg	monthly averaged concentrations in $\mathrm{g\,m^{-3}}$.

[†2] `http://code916.gsfc.nasa.gov/People/Chin/gocartinfo.html`

where *yyyymm* is the year and month (e.g., 200103), *XX* is the Gocart species, which can be either SU (sulfur), CC (carbonaceous), DU (dust), SS (sea-salt), and *vs* is the version (e.g., STD.tv12).

Gocart species may have further speciations:

- **SU** (sulfur): Total 4, 1-DMS, 2-SO2, 3-SO4, 4-MSA.
- **CC** (BC+OC): Total 4, 1-hydrophobic BC, 2-hydrophobic OC, 3-hydrophilic BC, 4-hydrophilic OC.
- **DU** (dust): Total 5, 1-Re=0.1-1, 2-Re=1-1.8, 3-Re=1.8-3, 4-Re=3-6, 5-Re=6-10 μm. The first group (0.1-1 μm) contains the following subgroups:
  - 0.10-0.18 μm (fraction = 0.01053)
  - 0.18-0.30 μm (fraction = 0.08421)
  - 0.30-0.60 μm (fraction = 0.25263)
  - 0.60-1.00 μm (fraction = 0.65263)
- **SS** (sea-salt): Total 4, 1-Re=0.1-0.5, 2-Re=0.5-1.5, 3-Re=1.5-5, 4-Re=5-10 μm.

The data format of Gocart files is "direct access binary, 32 bits, big endian". As an example, here is how they should be read in Fortran 77 language:

```
dimension Q(imx,jmx,lmx)
do k=1,nstep
 do n=1,nmx
  read(unit) nt1,nt2,nn,Q
 end do
enddo
```

where

- imx = total number of longitudinal grid (144),
- jmx = total number of latitudinal grid (91),
- lmx = total number of vertical layers (version dependent),
- nmx = total number of species (4 or 5, see species list above),
- nt1 = yyyymmdd after 2000 (year-month-day, e.g., 20010201), or yymmdd before 2000 (e.g., 970101)
- nt2 = hhmmss (hour-minute-second, e.g., 120000)
- nn = tracer number (see species list above)
- Q = 3-dimensional concentration of tracer nn
- nstep = total time step (e.g., in 200101, nstep=4*31 for 4-times/day, nstep=31 for daily average files, and nstep=1 for monthly average files).

Important

- If you plan to read Gocart data on your own, do not forget to translate files from big endian to little endian if necessary.
- The conventions and format of Gocart files may change in the future.

Fields resolution

The horizontal resolution of Gocart fields is 2 degree latitude $\times$ 2.5 degree longitude, except at the poles where latitudinal resolution is 1 degree. In other words the longitude interval is $[-180 : 2.5 : 177.5]$ (144 cells) and the latitude one is $[-89.5 - 88 : 2 : 8889.5]$ (91 cells).

The vertical resolution is given as a given number of vertical sigma levels. The number of vertical levels depends of the year :

- **1980-1995**: 20 sigma layers centered at 0.993936, 0.971300, 0.929925, 0.874137, 0.807833, 0.734480, 0.657114, 0.578390, 0.500500, 0.424750, 0.352000, 0.283750, 0.222750, 0.172150, 0.132200, 0.100050, 0.0730000, 0.0449750, 0.029000, 0.00950000
- **1996-1997**: 26 vertical sigma layers centered at 0.993935, 0.971300, 0.929925, 0.875060, 0.812500, 0.745000, 0.674500, 0.604500, 0.536500, 0.471500, 0.410000, 0.352500, 0.301500, 0.257977, 0.220273, 0.187044, 0.157881, 0.132807, 0.111722, 0.0940350, 0.0792325, 0.0668725, 0.0565740, 0.0447940, 0.0288250, 0.00997900
- **2000-2002**: 30 vertical sigma layers centered at 0.998547, 0.994147, 0.986350, 0.974300, 0.956950, 0.933150, 0.901750, 0.861500, 0.811000, 0.750600, 0.682900, 0.610850, 0.537050, 0.463900, 0.393650, 0.328275, 0.269500, 0.218295, 0.174820, 0.138840, 0.109790, 0.0866900, 0.0684150, 0.0539800, 0.0425750, 0.0335700, 0.0239900, 0.0136775, 0.00501750, 0.00053000

Gocart files processing

Gocart files are handled by `bc-gocart` program which takes 4 arguments:

```
./bc-gocart ../general.cfg bc-gocart-CC.cfg 200101.CC.STD.tv15.g.day 200101
```

where

- `../general.cfg` is the general configuration file,
- `bc-gocart-CC.cfg` is the configuration file for CC Gocart species,
- `200101.CC.STD.tv15.g.day` is the Gocart file
- `200101` is the date of Gocart file, this file corresponds to daily carbonaceous values during month of January 2001.

The gocart configuration file `bc-gocart-CC.cfg` provides all necessary informations to read Gocart fields and how to translate them into `polair3d` species.

	`[paths]`
`Temperature`	Meteorological file of temperature.
`Directory_bc`	Directory where output will be written.
	`[bc_input_domain]`

x_min	Minimum longitude in Gocart resolution.
y_min	Minimum latitude in Gocart resolution.
Delta_x	Gocart longitude resolution.
Delta_y	Gocart latitude resolution.
Nx	Number of grid cells in the longitude Gocart axe.
Ny	Number of grid cells in the latitude Gocart axe.
Nz	Number of Gocart vertical layers.
Sigma_levels	File where are written the center of Gocart sigma levels.
Scale_height	Scale height in meter.
Surface_pressure	Surface pressure in atm.
Top_pressure	Pressure at top of Gocart level (in atm).

There are two more sections in configuration file.

The first one is `[input_species]`. Each non blank line of this section corresponds to one speciation of Gocart species, e.g. CC is sub-divided in CC-1, CC-2, CC-3, CC-4. The range after the delimiter ":" is the aerosol size range (in SIμm) to which this sub-species apply. Most of the time this is the whole aerosol size range of `polair3d` model (e.g. $0.1 - 10.0$), but in the case of dust (DU) each sub-species may correspond to a precise part of the `polair3d` aerosol size range, see configuration file `bc-gocart-DU.cfg` for an illustration.

The second section is `[output_species]`. Each non blank line of this section corresponds to one aerosol species of `polair3d` model. The columns after ":" delimiter correspond to the Gocart sub-species. Therefore the number of line in previous section must equal the number of column after ":" delimiter. The numbers in these columns are the fraction (between $0.0 - 1.0$) of given Gocart sub-species that will contribute to given model species. As an example in `bc-gocart-CC.cfg` the first line

```
PBC:    1.      0.      1.      0.
```

means that sub-species CC-1 and CC-3 will fall into PBC `Polair3D` species, and nowhere else. In the same way the following line

```
PPOA:   0.      0.4     0.      0.4
```

means that PPOA species is composed of 40% of CC-2 and 40% of CC-4.

Important The Gocart files are proceeded month by month.

- The beginning date of computation is the one provided in `../general.cfg` if the beginning month is equal to the Gocart month, beginning of Gocart month otherwise.
- The end date of computation is provided by the length of file `Temperature`. If this length exceeds the Gocart month, the end date is set to end of Gocart month.
- If some boundary files already exist, the program `bc-gocart` will not overwrite them but append its result to each.

For example if you want to compute boundary conditions between 15th of April to 15th of June 2001, you would launch `bc-gocart` three times:

```
./bc-gocart ../general.cfg bc-gocart-CC.cfg 200104.CC.STD.tv15.g.day 200104
./bc-gocart ../general.cfg bc-gocart-CC.cfg 200105.CC.STD.tv15.g.day 200105
./bc-gocart ../general.cfg bc-gocart-CC.cfg 200106.CC.STD.tv15.g.day 200106
```

The file given in `Temperature` field of configuration file `bc-gocart-CC.cfg` must respectively start and end exactly at dates 2001-04-15 and 2001-06-15.

The python script `bc-gocart.py` provides an easy way to compute boundary conditions without worrying about how many times to launch `bc-gocart`. In the last example, one should simply launch:

```
./bc-gocart.py ../general.cfg 04 06
```

where 04 and 06 respectively stands for the first and last month to treat. Pay attention that some paths must be supplied inside this script (paths of Gocart configuration and data files) for it to work.

Remarks

Gocart **does not** provide any boundary conditions for nitrate and ammonia, you have to compute them on your own.

3.9 Preprocessing for Gaussian Models

3.9.1 Program `discretization`

The aim of this program is to discretize a line emission in the case of a continuous source (plume source) or an instantaneous one (puff source). It reads a line source given by two points or more, and gives in return the discretized source. The output data is a list of point sources whose coordinates have been calculated given the line coordinates and the number of points to discretize the line, or the source velocity in the case of a moving source (for puff sources only).

The program `discretization` is launched with one configuration file. The reference configuration file is `discretization.cfg`. It contains the following information:

	`[trajectory]`
`Trajectory_file`	Path to the data file that contains the line coordinates.
`Np`	Number of points to calculate on the discretized trajectory. Used only when the source is continuous or when it is not moving.
`Delta_t`	Time step to calculate the discretized trajectory in the case of a moving source.
	`[source]`
`Source_type`	Source type: `puff` or `continuous`.
`Species_name`	Name of the species emitted by the source (only one species for one line source).
	`[plume-source]`
`Rate`	Source rate (in mass per second) of the line source.
`Velocity`	Velocity of the gas or aerosol emitted by the source (in $\mathrm{m\,s^{-1}}$).
`Temperature`	Temperature of the gas or aerosol emitted by the source (Celsius degrees).
`Section`	Section of the source in $\mathrm{m^2}$.
	`[puff-source]`
`Quantity`	Total mass released on the line source (mass unit).

`Source_velocity`	Source velocity (in $km\,h^{-1}$) (0. for non mobile sources).
`tinit`	Release time for the first trajectory point (in s).
	`[output]`
`With_comment`	Are comments written?
`Source_file`	Path to the data file where the list of sources will be written.

The associated data file (reference: `line-emission.dat`) contains the coordinates of the line source to be discretized. The line source is a continuous line made of segments. Each segment is defined by two end points. The data file contains three columns corresponding to the coordinates (X, Y, Z in meters) of all end points. It contains at least the coordinates of two points.

This is an example of data file, defining a straight line emission between two points:

```
#X(m)   Y(m)    Z(m)
0.      0.     30.
20.     0.     30.
```

The output data file contains a list of point sources. All points have the same source data and their coordinates have been calculated by the program. It is presented as a list of sections named `[source]`, each section containing the coordinates and other data for one point source.

3.9.2 Programs `gaussian-deposition` and `gaussian-deposition_aer`

The aim of these programs is to calculate the scavenging coefficient and the deposition velocity of the species. The program `gaussian-deposition` is used when all species are gaseous species, and `gaussian-deposition_aer` is used when some or all species are aerosol species. The input data are meteorological data and species data, and the output file is a file containing meteorological data and the scavenging coefficients and deposition velocities of all species. This file can be used as input meteorological file for the programs `plume` and `puff` for gaseous species, or `plume_aer` and `puff_aer` in the case of aerosol species.

Program gaussian-deposition

Configuration File The program `gaussian-deposition` is launched with one configuration file and two input files. The configuration file contains the path to the two input files and to the output file. The reference configuration file is `gaussian-deposition.cfg`. It contains the following information:

	`[data]`
`Species`	Path to the data file that contains the species data.
`Meteo`	Path to the data file that contains the meteorological data.
	`[scavenging]`
`Type`	Parameterization to be used to calculate the scavenging coefficients.
	`[deposition]`
`Type`	Parameterization to be used to calculate the deposition velocities.
	`[output]`

`With_comment`	Are comments written in the output file? (put yes or no).
`Output_file`	Path to the file where the output data are written.

The parameterization type for the scavenging coefficient can be chosen between:

- `none`: the scavenging coefficient is set to 0. for all species
- `constant`: the scavenging coefficient is constant for one given species and entered in the species file.
- `belot`: the scavenging coefficient is calculated with a Belot parameterization. In that case, the input data are a rainfall rate given in the meteorological data file, and coefficients a and b given for each species in the species file.

Concerning the deposition velocity, the type can be chosen between:

- `none`: the deposition velocity is set to 0. for all species
- `constant`: the deposition velocity is constant for one given species and is given in the species file.

Input Files There are two input data files for this program: the meteorological data file (reference: `meteo.dat`) and the species file (reference: `species.dat`).

1. Meteorological data file: it contains as many sections as there are meteorological situations. For each situation, meteorological data are given: the temperature (in Celsius degrees), the wind angle (in degrees), the wind speed (in $\mathrm{m\,s^{-1}}$), the inversion height (in m) and the stability class which is given by a letter between a and f (based on the Pasquill stability classes). These five data must always be provided (the inversion height is set to 0. if not known) and they are written in the output file which will be the meteorological data file of the main program. Other meteorological data might be needed, depending on the chosen parameterization. Currently, the only parameterization that needs other information is the Belot parameterization. If the type `belot` is chosen for the calculation of the scavenging coefficient, a rainfall rate must be provided (in $\mathrm{mm\,h^{-1}}$). If the chosen type is `constant` or `none`, the rainfall rate or other information can be provided but will be ignored by the program. So, the meteorological data file finally looks like this:

```
[situation]

# Temperature (Celsius degrees)
Temperature = 10.

# Wind angle (degrees)
Wind_angle = 30.

# Wind speed (m/s)
Wind = 3.0
```

```
#Inversion height (m)
Inversion_height = 1000.

# Stability class
Stability = D

# Rainfall rate (mm/hr)
Rainfall_rate = 1.
```

In this example, there is only one meteorological situation described. Others can be added simply by adding similar sections `[situation]` at the end of the file.

2. Species data file: it contains several sections, but not all are needed for the preprocessing. The needed sections are:

   - `[species]` Contains the list of all species.
   - `[scavenging]` Contains the list of the species for which scavenging occurs. The scavenging coefficient of the others is set to 0.
   - `[deposition]` Contains the list of the species for which deposition occurs. The deposition velocity of the others is set to 0.
   - `[scavenging_constant]` This section is needed when the type of parameterization chosen for the scavenging is `constant`. It contains the name of a species followed by the value of its scavenging coefficient (in s^{-1}). Only one species per line must be provided. All species listed in the section `[scavenging]` must be present (the order is not important), the others will be ignored.
   - `[scavenging_belot]` This section is needed when the type of parameterization chosen for the scavenging is `belot`. It contains the name of a species followed by two values corresponding to the coefficients a and b respectively in the Belot parameterization. Only one species per line must be provided. All species listed in the section `[scavenging]` must be present, the others will be ignored.
   - `[deposition_constant]` This section is needed when the type of parameterization chosen for the deposition is `constant`. It contains the name of a species followed by the value of its deposition velocity (in $m\,s^{-1}$). Only one species per line must be provided. All species listed in the section `[deposition]` must be present, the others will be ignored.

   A species file might look like this:

```
[species]

Caesium       Iodine


[scavenging]

Iodine        Caesium

[deposition]
```

```
Caesium        Iodine


[scavenging_constant]

Caesium: 1.e-4
Iodine: 1.e-4


[scavenging_belot]

Caesium: 2.8e-05  0.51
Iodine: 7e-05  0.69


[deposition_constant]

Caesium: 0.05e-2
Iodine: 0.5e-2
```

Output File The output data file contains as many sections as there are meteorological situations. Each section `[situation]` contains the temperature, wind angle, wind speed, inversion height and stability class that are provided. In addition, it contains the list of all species followed by their scavenging coefficient, and the list of all species followed by their deposition velocity. It looks like this:

```
[situation]

# Temperature (Celsius degrees)
Temperature = 10

# Wind angle (degrees)
Wind_angle = 30.

# Wind speed (m/s)
Wind = 3.

# Inversion height (m)
Inversion_height = 1000

# Stability class
Stability = D

# Scavenging coefficient of the species (s^-1)
 Scavenging_coefficient =
 Caesium  6.36257e-05  Iodine  0.000212514

# Deposition velocity of the species (m/s)
```

```
Deposition_velocity =
Caesium  0.0005  Iodine  0.005
```

Program gaussian-deposition_aer

The program `gaussian-deposition_aer` works the same way as the program `gaussian-deposition`, except that there are some more information specific to the aerosol species. The input and output files are the same as described in the section about `gaussian-deposition`, so in this section we will only describe the data that are added to the files described previously. One input file is needed in addition to the meteorological data and species data files. It is the diameter file (reference: `diameter.dat`) which contains the diameters of the aerosol particles.

Configuration File In the configuration file, the following information are added:

	`[data]`
`Diameter`	Path to the data file that contains the particle diameters.
	`[scavenging]`
`Type_aer`	Parameterization to be used to calculate the scavenging coefficients for aerosol species.
`Value`	Values to be used for a Slinn parameterization (choose between `best_estimate` and `conservative`.
	`[deposition]`
`Type_aer`	Parameterization to be used to calculate the deposition velocities for aerosol species.

The parameterization type for the scavenging coefficient of aerosol species can be chosen between:

- `none`: the scavenging coefficient is set to 0. for all aerosol species
- `constant`: the scavenging coefficient is constant for one given diameter and entered in the species file.
- `slinn`: the scavenging coefficient is calculated with a Slinn parameterization. In that case, the only input data that are used are the rainfall rate and the particle diameters.

Concerning the deposition velocity, the type can be chosen between:

- `none`: the deposition velocity is set to 0. for all species
- `constant`: the diffusive part of the deposition velocity is constant for one given diameter and entered in the species file. The gravitational settling velocity is calculated for each particle, given the density and the diameter (provided in the species file) and the pressure and temperature (provided in the meteorological data file).

Input Files

1. Meteorological data file: it is the same as the one for `gaussian-deposition`. If the parameterization type for the deposition velocity calculation is `constant`, the pressure must

be provided (in Pa).

2. Diameter file: it contains the list of particle diameters (in µm). The first number is the diameter of index 0, the second of index 1, and so on. This is an example of diameter file:

```
#Diameter (micrometer)
[diameter]
0.1
1.
```

The diameter of index 0 corresponds to the value 0.1 µm, the diameter of index 1 to the value 1. µm and so on. When referring to a given diameter in the other data files, one has to give the corresponding index. Note that there is only one diameter file for all aerosol species. Therefore all particulate species are assumed to have the same diameter distribution. The diameter file can also be the main configuration file. In that case, the section `[diameter]` is simply added to the main configuration file.

3. Species file: it is the same as described before, but the sections described for `gaussian-deposition` concern only gaseous species. All data concerning aerosol species are added in the following sections:

   - `[aerosol_species]` Contains the list of all aerosol species.
   - `[scavenging_constant_aer]` This section is needed when the type of parameterization chosen for the scavenging for aerosol species is `constant`. In that case, the scavenging coefficient is assumed to be constant for one particle diameter. So the section contains the index of one diameter followed by the corresponding value of the scavenging coefficient (in s^{-1}). Only one diameter per line must be provided.
   - `[deposition_constant_aer]`This section is needed when the type of parameterization chosen for the deposition of aerosol species is `constant`. It contains the index of a diameter followed by the value of its deposition velocity (in $m\,s^{-1}$). Only one diameter per line must be provided.
   - `[density_aer]` It contains the density of the aerosol species. That is, the name of each aerosol species followed by the corresponding density (in $kg\,m^{-3}$). Only one species per line must be provided. This section is needed in order to calculate the gravitational settling velocity of a particle. The calculated deposition velocity of one species of a given diameter is therefore a combination of the diffusive part given in the section `[deposition_constant_aer]` and the gravitational settling velocity calculated by the program.

Note that while some gaseous species might not be concerned by scavenging or deposition, the loss processes are assumed to occur for all aerosol species. Therefore, there is no need of a section containing the species for which scavenging or deposition occur in the case of aerosol species, as it is the case for gaseous species. Here is an example of species file containing the sections dedicated to aerosol species:

```
[aerosol_species]

aer1
```

```
aer2
aer3


[scavenging_constant_aer]

# Scavenging coefficient for aerosol species ( Unit: seconds^(-1) )
# Depends on the diameter (first value: diameter index in file diameter.dat).
# Only one diameter per line.

0: 1.e-4
1: 2.e-4


[deposition_constant_aer]

# Dry deposition velocity (diffusive part) of the species (Unit: m/s)
# Depends on the diameter
# Only one diameter per line.

0: 0.05e-2
1: 0.5e-2


[density_aer]

# Particle density (aerosol species) (kg/m^3)
# Only one species per line.

aer1: 1.88
aer2: 1.
aer3: 4.93
```

Output File The output file is the same file as the one for `gaussian-deposition`, except that the scavenging coefficients and deposition velocities of aerosol species are also written. One coefficient corresponds to a given species of a given diameter. It is written as "species-name"-"diameter-index" followed by the value of the corresponding scavenging coefficient (or deposition velocity). The following example corresponds to a case with two gaseous species named "gas1" and "gas2" and three aerosol species named "aer1", "aer2" and "aer3". The diameter file is the same as displayed before, that is, contains two diameters. The output file looks like this:

```
[situation]

# Temperature (Celsius degrees)
Temperature = 10

# Pressure (Pa)
Pressure = 101325
```

```
# Wind angle (degrees)
Wind_angle = 30

# Wind speed (m/s)
Wind = 3

# Inversion height (m)
Inversion_height = 1000

# Stability class
Stability = D

# Scavenging coefficient of the gaseous species (s^-1)
Scavenging_coefficient =
gas1  0.0001    gas2  0.0001

# Deposition velocity of the gaseous species (m/s)
 Deposition_velocity =
 gas1  0.0005     gas2  0.005

# Scavenging coefficient of the aerosol species (s^-1)
 Scavenging_coefficient_aer =
 aer1-0  5.95238e-05      aer1-1  5.95238e-05    aer2-0  5.95238e-05
 aer2-1  5.95238e-05      aer3-0  5.95238e-05    aer3-1  5.95238e-05

# Deposition velocity of the aerosol species (m/s)
 Deposition_velocity_aer =
 aer1-0  2.11708     aer1-1  6.69479      aer2-0  1.54404
 aer2-1  4.88268     aer3-0  3.42833      aer3-1  10.8413
```

The value following “aer1-0” corresponds to the calculated coefficient for the species “aer1” and the diameter of index 0, that is, in the case of our diameter file, the diameter equal to 0.1 µm. The value following “aer1-1” corresponds to the coefficient for the species “aer1” and the diameter of index 1, that is, equal to 1 µm, and so on.

Chapter 4

Drivers

4.1 BaseDriver

BaseDriver is configured with a file which contains the displaying options for the simulation.

[display]	
`Show_iterations`	If activated, each iteration is displayed on screen.
`Show_date`	If activated, the starting date of each iteration is displayed on screen in format `YYYY-MM-DD HH:II` (notations from Section 2.2.7).

4.2 PlumeDriver

It is the driver dedicated to the Gaussian plume model. The associated configuration file is the same as the one for the BaseDriver, and it is usually part of the model configuration file described in Section 5.1. The associated input data file describes the meteorological data (reference: `gaussian-meteo.dat`) for gaseous species and `gaussian-meteo_aer.dat` for aerosol and/or gaseous species. The meteorological data file contains the meteorological data that are needed. It can be the output file of the preprocessing program `gaussian-deposition`.

The meteorological data file describes one or several meteorological situations. For each situation, the driver calls the model to calculate the concentrations, that is, the stationary solution for the given meteorological situation. It is associated with two models: the GaussianPlume model for gaseous species only (described in Section 5.1) and the GaussianPlume_aer model which is the same model for aerosol and/or gaseous species (see Section 5.2).

4.3 PuffDriver

It is the driver dedicated to the Gaussian puff model. The associated configuration file is the same as the one for the BaseDriver, and it is usually part of the model configuration file described in Section 5.3. The associated input data file describes the meteorological data. It is the same file as for the plume model.

For each meteorological situation, the driver calculates the concentrations that depend on time. That is, for a given situation, it makes a loop on time and calls the model at each time step to calculate the current concentrations. It is associated with two models: the GaussianPuff model for gaseous species only (described in Section 5.3) and the GaussianPuff_aer model which is the same model for aerosol and/or gaseous species (see Section 5.4).

4.4 StationaryDriver

This driver, as the Gaussian drivers presented before, is used to perform a simulation at local scale, the only difference being that in that case an Eulerian model is used.

An additional section `[stationary]` is necessary in the configuration file:

	`[stationary]`
`Nt`	Number of stationary steps.
`Delta_t`	Time-step between stationary steps.

4.5 OptimalInterpolationDriver

It is the driver dedicated to data assimilation applications using optimal interpolation algorithm. The associated configuration file is an extension of that of BaseDriver, and it is usually part of the model configuration file exemplified in Section 5.8. It has an additional section `[observation_management]` similar to what can be seen below:

```
[observation_management]

# For configuration file, choose between observation.cfg
# and observation-sim.cfg.
Configuration_file: example/assimilation/observation.cfg
```

The value of `Configuration_file` can be set to `observation.cfg` if you use `GroundObservationManager` (see Section 4.7.1) and to `observation-sim.cfg` if you use `SimObservationManager` (see Section 4.7.2).

The optimal interpolation algorithm estimates model state status by minimizing the error variance of the estimation (called *analysis* in data assimilation terminology). It searches for a linear combination between *background* state (model simulations) and the *background departures*. The background departures are defined as the discrepancies between observations and background state. It involves with observation managements (described in Section 4.7) and storage managements of forecast and analysis results (see for instance Section 4.6.4).

4.6 Output Savers

4.6.1 BaseOutputSaver

The saver `BaseOutputSaver` is configured with a file that contains one or several sections `[save]`. Each section is associated with one element of a list of output-saver units managed by `BaseOutputSaver`.

According to the value of `Type` in every section, different saver units are called. Note however that a `group` attribute can be set in `BaseOutputSaver` (the default being `all`, and the other choices being `forecast` and `analysis`) and that only savers with the same group are called.

Some parameters must be provided for any kind of savers:

`Species`	Chemical species to be saved. If it is set to `all`, concentrations for all species are saved.

Date_beg	The date from which the concentrations are saved. If concentrations are averaged, the first step at which concentrations are actually saved if not Date_beg, but Date_beg plus the number of steps over which concentrations are averaged. If the value - 1 is supplied, Date_beg is set at the start of the simulation.
Date_end	The last date at which concentrations may be saved. If the value - 1 is supplied, Date_end is set at the end of the simulation.
Interval_length	The number of steps between saves.
Type	The type of saver, see Table 4.4 for details.
Output_file	The full path of output files, in which &f will be replaced by the name of the chemical species. Note that the directory in which the files are written must exist before the simulation is started.

Note that Species, Date_beg, Date_end, Interval_length must appear before Type. After Type, put additional options relevant for the chosen output saver.

Here is a list of all types of saver units available at the moment:

Table 4.4: Types of saver

domain	To save entire vertical layers.
domain_aer	The same as domain but for aerosol species.
domain_assimilation	The same as domain but for data assimilation applications.
nesting	To perform nested simulations.
nesting_aer	The same as nesting but for aerosol species.
subdomain	To save concentrations only for an horizontal subdomain.
subdomain_aer	The same as subdomain but for aerosol species.

4.6.2 SaverUnitDomain and SaverUnitDomain_aer

The output saver SaverUnitDomain defines an output-saver unit when Type is set to "domain"and requires additional parameters presented in the table below.

Levels	A list of integers that determines the vertical layers to be saved. Note that 0 is the first layer. Remember that the heights you specified in the file levels.dat are those of the level interfaces, while concentration are saved in the middle of each levels.
Averaged	Should concentrations be averaged over Interval_length? If not, instantaneous concentrations are saved.
Initial_concentration	Should initial concentrations be saved? This option is only available if concentrations are not averaged.

For aerosol species, the saver should be SaverUnitDomain_aer and the Type "domain_aer". The section [save] is very similar to the one for gaseous species, except that you have to specify for which diameters the concentrations are saved. Hence, the list of species to be saved looks like this:

```
Species: aer1_{0} aer 1_{2} aer2_{0-1}
```

In that case, the species named "aer1" is to be saved for the diameter of indices 0 and 2, and "aer2" for the diameters of indices 0 and 1.

In `Output_file`, `&f` will be replaced by the species name and `&n` by the bin index. You can use any symbol which is not a delimiter (or even nothing) to separate the species name from the bin index, even though `&f_&n.bin` is the advised form.

If `Species` is set to "all" the concentrations will be saved for all aerosol species and for all diameters.

4.6.3 SaverUnitSubdomain and SaverUnitSubdomain_aer

These saver units allow the user to save concentrations only over an horizontal subdomain (for example, if they perform a simulation over the whole of Europe but only want the concentrations over one country or region). Their `Type` is "subdomain" and "subdomain_aer" respectively. The user must provide between which indices for x and y they want to save concentrations. The specific parameters for these saver units are:

`Levels`	A list of integers that determines the vertical layers to be saved. Note that 0 is the first layer. Remember that the heights you specified in the file `levels.dat` are those of the level interfaces, while concentration are saved in the middle of each levels.
`Averaged`	Should concentrations be averaged over `Interval_length`? If not, instantaneous concentrations are saved.
`Initial_concentration`	Should initial concentrations be saved? This option is only available if concentrations are not averaged.
`i_min`	Minimum latitude index of the subdomain.
`i_max`	Maximum latitude index of the subdomain.
`j_min`	Minimum longitude index of the subdomain.
`j_max`	Maximum longitude index of the subdomain.

4.6.4 SaverUnitDomain_assimilation

The output saver `SaverUnitDomain_assimilation` defines an output-saver unit similar to `SaverUnitDomain`, except that it requires additional parameters presented in the table below.

`Date_file`	The full path name of the file that stores the date sequences of the assimilation results.

The `group` attribute of the output saver `SaverUnitDomain_assimilation` is set to "analysis", whereas the `group` attributes of other saver units are set to "forecast" by default. Its `Type` is "domain_assimilation".

4.6.5 SaverUnitNesting and SaverUnitNesting_aer

The saver units `SaverUnitNesting` and `SaverUnitNesting_aer` are used to perform nested simulations. That means that the results of a first simulation on a large domain are interpolated and saved at the boundary of a subdomain and are then used as boundary conditions for a second simulation on the subdomain. If the saver unit is of `Type` "nesting" or "nesting_aer", the additional parameters needed in the section `[save]` are presented in the table below.

`x_min`	Origin of the subdomain along x.
`Delta_x`	Step along x for the subdomain.
`Nx`	Number of points along x for the subdomain.
`y_min`	Origin of the subdomain along y.

Delta_y	Step along y for the subdomain.
Ny	Number of points along y for the subdomain.
levels	File giving the interfaces of the layers for the subdomain.
Nz	Number of layers in the subdomain.

In Output_file &f and &n are replaced as for SaverUnitDomain or SaverUnitDomain_aer and &c is replaced by the direction along which the boundary conditions were interpolated (that means that &c is replaced by x, y or z).

4.7 Observation Managers

The observation managers deal with available observational data at different locations and dates. These managers are designed to prepare for applications related to observation treatments, especially for data assimilation. The observation operator are implemented for the mapping from observation space into model space. For a given date, these managers retrieve observation data values and the corresponding statistical information, e.g. observational error covariances.

4.7.1 GroundObservationManager

The GroundObservationManager is dedicated to ground observation managements.

	[general]
Species	Name of observed species. The current version deals with only one observed species.
Error_variance	Error variance for the observed species.
With_spatial_interpolation	Should observations be interpolated at adjacent model grid points?
With_perturbation	Should the observation be perturbed?
Perturbation_scale	If With_perturbation is set to "yes", gives the amplitude of the perturbation.
	[stations]
Nstations	Total number of stations.
Stations_file	File containing station information (code, name, latitude, longitude and altitude). &s in path names is replaced by species name specified in [general] section.
Input_directory	Directory where the observations are stored.

4.7.2 SimObservationManager

The SimObservationManager is dedicated to synthetic observation managements. Library NewRan is needed for random number generations. Note that NewRan is not included in the distribution, and it is the user's duty to install NewRan. The associated configuration file is an extension of that of GroundObservationManager. The additional sections are mainly for data specifications of the binary data files.

	[simulation_manager]
Simulation_option	Specifies how observations are provided. The current version deals only with observations at ground stations.

`Input_file`	Files containing the observation data. They usually are generated by certain reference run of Polair3D. `&s` in path names is replaced by species name.
`Date_min`	Starting date for the simulation results in data files.
`Delta_t`	Time step in seconds for the simulation results in data files.
`Levels`	Levels for the simulated data in files.
`Initial_concentration`	Flag that indicates whether initial concentrations are included in data file.

Chapter 5

Models

There are three major types of models: Gaussian models (see Section 5.1, 5.2, 5.3 and 5.4), Polair models (see Section 5.5, 5.6, and 5.7) and Castor models (see Section 5.9). All variants of a model have the same principles but can deal with various applications and phenomena.

Polair models were the first implemented in Polyphemus. They allow, as well as Castor models, to compute the advection and diffusion of pollutants at a large scale and can integrate various additional phenomena (such as photochemical chemistry or deposition). Gaussian models have been added to perform simulation at a local scale of the effect of a continuous (plume) or instantaneous (puff) source of pollutant.

As for now, Castor models only deal with gaseous species, while the other models deal with gaseous or aerosol species.

5.1 GaussianPlume

Model `GaussianPlume` is the Gaussian plume model for gaseous species only. The associated program to be run is `plume` and it is configured with one configuration file (`plume.cfg`) and four data files (`plume-source.dat`, `plume-level.dat`, `gaussian-meteo.dat` and `gaussian-species.dat`). The configuration file provides the paths to the four other files. Basically, given a series of continuous point sources, it calculates the concentration of each species along a specified grid. There are several output files, one for each species, that are binary files. The way results are saved is described in an additional configuration file which corresponds to the file described in Section 4.6 (reference: `plume-saver.cfg`).

In these configuration files, there are entries that are not relevant for the Gaussian model but that must be provided anyway. In descriptions of configuration files (below), they are described as `irrelevant`.

5.1.1 Configuration File: `plume.cfg`

	`[domain]`
`Date_min`	**Irrelevant.** Provide a date.
`Delta_t`	**Irrelevant.** Provide any number.
`Nt`	**Irrelevant.** Provide an integer.
`x_min`	Abscissa in meter of the center of the lower-left cell.
`Delta_x`	Step length along x (in m).
`Nx`	Number of cells along x (integer).
`y_min`	Ordinate in meter of the center of the lower-left cell.

`Delta_y`	Step length along y (in m).
`Ny`	Number of cells along y (integer).
`Nz`	Number of vertical levels (integer).
`Vertical_levels`	Path to the file that defines vertical levels heights.
`Land_category`	Land category (choose between `rural` and `urban`).
`Time`	Choose whether it is nighttime (`night`) or daytime (`day`). Relevant only when there is biological decay.
`Species`	Path to the file that defines involved species.
	`[gaussian]`
`With_plume_rise`	Is plume rise taken into account?
`With_radioactive_decay`	Is radioactive decay taken into account?
`With_biological_decay`	Is biological decay taken into account?
`With_scavenging`	Is scavenging taken into account?
`With_dry_deposition`	Is dry deposition taken into account?
`File_meteo`	Path to the file containing the meteorological data.
`File_source`	Path to the file that describes the sources.
	`[deposition]`
`Deposition_model`	Model used to take dry deposition into account (`Chamberlain` for Chamberlain model, `Overcamp` for Overcamp model).
`Nchamberlain`	Number of points to calculate the Chamberlain integral (integer). Relevant only when dry deposition with Chamberlain model is taken into account.
	`[output]`
`Configuration_file`	Path to the configuration for the output saver.

Note: The Chamberlain integral for the calculation of dry deposition is discretized and approximated as a sum. The integer that is provided corresponds to the number of terms of the sum in the plume model. In the puff model, it is incremented at each time step, so as to have a number of points consistent with the range of the integral (that is, not to have too many points to discretize an integral whose range is very small).

5.1.2 Source Description: `plume-source.dat`

Sources are described in a single configuration file containing as many sections as there are sources. Each section named `[source]` is associated with a new source. Each section contains the following information: (1) the emission rate (in mass per seconds – the mass unit does not matter: the model will stick to it), (2) the velocity of emitted pollutants ($\mathrm{m\,s^{-1}}$), (3) the temperature of pollutants when emitted ($^{\circ}$C), (4) the section area (in $\mathrm{m^2}$) of the source (most likely a stack), (5) the abscissa of the source (m), (6) the ordinate of the source (m), (7) the height of the source (m), and (8) the species that is emitted.

A typical source file looks like this:

```
[source]

# Source coordinates (meters)
Abscissa: 100.
Ordinate: 100.
```

```
Altitude: 0.5
# Species name
Species_name: Iodine

# Source rate (mass/s)
Rate = 56.5
# Source velocity (m/s)
Velocity = 10.1
# Source temperature (Celsius degrees)
Temperature = 60.
# Source section (m^2)
Section = 5.725
```

In this example, only one section is provided, but other sources may be added simply by adding the corresponding sections at the end of the file. One species may have several sources. The source file can contain a list of point sources provided by the user or a discretized line source. In that case, it corresponds to the output file of the discretization preprocessing program `discretization`.

5.1.3 Vertical Levels: `plume-level.dat`

Vertical levels are defined in a single data file. They are defined by their interfaces. This means that the file contains `Nz+1` heights, where `Nz` is the number of levels specified in the main configuration file. The concentrations are computed at layers mid-points.

5.1.4 Species: `gaussian-species.dat`

Species are listed in the section `[species]` of a data file (the same as the species data file used in the preprocessing program `gaussian-deposition`, see Section 3.9.2). When radioactive or biological decay is taken into account, a section containing the half-life times of the species has to be provided. The section `[radioactive_decay]` contains the list of all species followed by their half-life time in days (put 0. in the case of non-radioactive species). Provide only one species per line. The section `[biological_decay]` contains two values following each species name, the first corresponding to its half-life time (in s) during daytime and the second to the value during nighttime (put 0. in the case of non biological species). Here is an example:

```
[species]

# List of the species
Caesium     Iodine    bio1


[radioactive_decay]

# Half-life of the species (Unit: days)
# 0 coresponds to non-radioactive species
Caesium: 1.1e4
Iodine: 8.04
bio1: 0.
```

```
[biological_decay]

# Half-life of the species ( Unit: seconds )
# First value: day, second value: night
# 0 corresponds to non-radioactive species.
Caesium: 0. 0.
Iodine:  0. 0.
bio1: 1000 500
```

In that case we have two radioactive species, "Caesium" and "Iodine", and one biological species, "bio1".

If scavenging is taken into account, sections `[scavenging]` and `[scavenging_constant]` must be added. The section `[scavenging]` contains the name of all species for which scavenging occur and `[scavenging_constant]` their constants in s^{-1}.

5.2 GaussianPlume_aer

It is the Gaussian plume model for aerosol species. The corresponding program is `plume_aer`. It can be run when there are aerosol species only, or both aerosol and gaseous species. It takes the same input files as the Gaussian plume model, except that they contain in addition some sections dedicated to aerosol species. It takes in addition another input file that describes the diameters of particles (file `diameter.dat` already described in Section 3.9.2). The output files are binary files, one for each gaseous species and one for each couple (aerosol species, diameter). The way results are saved is described in an additional configuration file (reference: `plume-saver_aer.cfg`) described in Section 4.6.

5.2.1 Configuration File: `plume_aer.cfg`

It is exactly the same file as the configuration file described in Section 5.1. The only data that may differ are the paths to the input files.

5.2.2 Source Description: `plume-source_aer.dat`

It is the same file as the source file for gaseous species, except that obviously some (or all) emitted species will be particulate species. The corresponding sections are named `[aerosol_source]`.

5.2.3 Vertical Levels: `plume-level.dat`

It is the same file as in Section 5.1.

5.2.4 Species: `gaussian-species_aer.dat`

The section `[species]` lists the gaseous species, and the section `[aerosol_species]` lists the aerosol species. In the case of radioactive or biological decay, the sections are the same as described in Section 5.1 and contain the half-life times of both gaseous and aerosol species.

5.2.5 Diameters: `diameter.dat`

See Section 3.9.2.

5.3 GaussianPuff

Model `GaussianPuff` is the Gaussian puff model for gaseous species only. The associated program to be run is `puff` and it is configured with one configuration file (`puff.cfg`) and four data files (`puff.dat`, `puff-level.dat`, `gaussian-meteo.dat` and `gaussian-species.dat`). The configuration file provides the paths to the four other files. Basically, given a series of instantaneous puffs emitted at different times, it calculates the concentration of each species along a specified grid. There are several output files, one for each species, that are binary files. (same as in the Gaussian plume model, and fully described in Section 4.6).

5.3.1 Configuration File: `puff.cfg`

	`[display]`
`Show_date`	**Irrelevant.** Provide any Boolean.
	`[domain]`
`Date_min`	**Irrelevant.** Provide any date (see Section 2.2.7).
`Delta_t`	Time step of the simulation (in seconds).
`Nt`	Number of time steps (integer).
`x_min`	Abscissa in meter of the center of the lower-left cell.
`Delta_x`	Step length along x (in m).
`Nx`	Number of cells along x (integer).
`y_min`	Ordinate in meter of the center of the lower-left cell.
`Delta_y`	Step length along y (in m).
`Ny`	Number of cells along y (integer).
`Nz`	Number of vertical levels (integer).
`Vertical_levels`	Path to the file that defines vertical levels heights.
`Land_category`	Land category (choose between `rural` and `urban`).
`Time`	Choose whether it is nighttime (`night`) or daytime (`day`). Relevant only when there is biological decay.
`Species`	Path to the file that defines involved species.
	`[gaussian]`
`With_radioactive_decay`	Is radioactive decay taken into account?
`With_biological_decay`	Is biological decay taken into account?
`With_scavenging`	Is scavenging taken into account?
`With_dry_deposition`	Is dry deposition taken into account?
`File_meteo`	Path to the file containing the meteorological data.
`File_puff`	Path to the file that contains the puff data.
	`[deposition]`
`Deposition_model`	Model used to take dry deposition into account (`Chamberlain` for Chamberlain model, `Overcamp` for Overcamp model)
`Nchamberlain`	Number of points to calculate the Chamberlain integral (integer). Relevant only when dry deposition with Chamberlain model is taken into account.
	`[output]`
`Configuration_file`	Path to the configuration for the output saver.

5.3.2 Puff Description: `puff.dat`

Puffs are described in a single configuration file containing as many sections as there are puffs. Each section named `[source]` is associated with a new source. Each section contains the following information: (1) the time when the puff is released (s) (from the beginning of the simulation) (2) the total mass emitted (in mass unit – the mass unit does not matter: the model will stick to it),(3) the abscissa of the point of emission (m), (4) the ordinate of the point of emission (m), (5) the height of the point of emission (m), and (6) the species that is emitted.

```
[source]

# Source coordinates (meters)
Abscissa: 0.
Ordinate: 5.
Altitude: 25.
# Species name
Species_name: Iodine

# Release time (seconds)
Release_time: 0.
# Total mass released (mass)
Quantity: 1.
```

One species may have several puffs. The puff file can contain a list of puffs provided by the user or a discretized line source or trajectory. In that case, it corresponds to the output file of the discretization preprocessing program `discretization`.

5.3.3 Vertical Levels and Species

They are exactly the same file as those described in Section 5.1.

5.4 GaussianPuff_aer

It is the Gaussian puff model for aerosol species. It can be run when there are aerosol species only, or both aerosol and gaseous species. It takes the same input files as the Gaussian puff model, except that they contain in addition some sections dedicated to aerosol species. It takes in addition another input file that describes the diameters of particles (file `diameter.dat` already described in the Section 3.9.2). The output files are binary files, one for each gaseous species and one for each couple (species, diameter).

5.4.1 Configuration File: `puff_aer.cfg`

It is exactly the same file as the configuration file described in Section 5.3. The only data that may differ are the paths to the input files.

5.4.2 Source Description: `puff_aer.dat`

It is the same file as the puff file for gaseous species described in Section 5.3, except that obviously some (or all) emitted species will be particulate species. The corresponding sections are named `[aerosol_source]`.

5.4.3 Vertical Levels, Species and Diameters

Vertical level file has been described in Section 5.1 and diameter files is the same as in Section 3.9.2. Species file is the same file as described for the plume model for aerosol species (Section 5.2.4).

5.5 Polair3DTransport

The model Polair3DTransport is configured with three configuration files (`polair3d.cfg`, `polair3d-data.cfg` and `polair3d-saver.cfg`) and two data files (`levels.dat` and `species.dat`). The main configuration file (`polair3d.cfg`) provides the paths to the four other files.

5.5.1 Main Configuration File: `polair3d.cfg`

	`[domain]`
`Date_min`	Starting date in any legal format (see Section 2.2.7). The date can therefore include seconds.
`Delta_t`	Time step in seconds.
`Nt`	Number of iterations of the simulation (integer).
`x_min`	Abscissa of the center of the lower-left cell. Provide a longitude (in degrees) or, in case Cartesian coordinates are chosen, an abscissa in meters.
`Delta_x`	Step length along x, in degrees (longitude) or in meters (for Cartesian coordinates).
`Nx`	Number of cells along x (integer).
`y_min`	Ordinate of the center of the lower-left cell. Provide a latitude (in degrees) or, in case Cartesian coordinates are chosen, an ordinate in meters.
`Delta_y`	Step length along y, in degrees (latitude) or in meters (for Cartesian coordinates).
`Ny`	Number of cells along y (integer).
`Nz`	Number of vertical levels (integer).
`Vertical_levels`	Path to the file that defines vertical levels interfaces.
`Cartesian`	If activated, coordinates are Cartesian and in meters. Otherwise, coordinates are latitudes and longitudes in degrees.
`Species`	Path to the file that defines involved species and their chemical properties.
	`[options]`
`With_advection`	Are species advected?
`With_diffusion`	Are species diffused?
`With_air_density`	If activated, vertical wind is diagnosed from $\mathrm{div}(\rho V) = 0$ where ρ is the air density and V the wind, and the diffusion term is $\mathrm{div}\left(\rho K \nabla \frac{c}{\rho}\right)$ where c is the concentration and K is the diffusion matrix. If this option is not activated, it is assumed that ρ is constant and therefore disappears from the previous equations.
`With_initial_condition`	Are initial conditions provided for given species? If not, initial concentrations are set to zero.

`With_boundary_condition`	Are boundary conditions available for given species?
`With_deposition`	Is dry deposition taken into account?
`With_point_emission`	Are point emissions provided?
`With_surface_emission`	Are emissions at ground provided?
`With_volume_emission`	Are volume emissions provided?
`Scavenging_model`	Which scavenging model is applied? If `none`, the scavenging is not taken into account. Otherwise, the following model is applied: `constant` for constant scavenging coefficient, `belot` for the Belot model (of the form $a\,{p_0}^b$, where p_0 is the rain intensity in $\mathrm{mm\,h^{-1}}$) or `microphysical` for the scavenging model based on microphysical properties of species.
	`[data]`
`Data_description`	Path to the configuration file that describes input data.
`Horizontal_diffusion`	Horizontal diffusion coefficient in $\mathrm{m^2\,s^{-1}}$.
`Isotropic_diffusion`	If activated, horizontal diffusion is set equal to vertical diffusion.
	`[output]`
`Configuration_file`	Path to the configuration for the output saver.

5.5.2 Data Description: `polair3d-data.cfg`

This configuration file describes input data files (binary files). It is divided into sections: for deposition, for meteorological fields, etc. A section roughly looks like this:

```
[meteo]

Date_min: 2004-08-09
Delta_t = 10800.

Fields: MeridionalWind ZonalWind Temperature Pressure Rain CloudHeight Attenuation\
SpecificHumidity
Filename: /u/cergrene/a/ahmed-dm/TestCase-1.0/data/meteo/&f.bin

VerticalDiffusion: /u/cergrene/a/ahmed-dm/TestCase-1.0/data/meteo/Kz_TM.bin
```

It is assumed that all binary files start at the same date, and this date is `Date_min` (see dates formats in Section 2.2.7). The time step is `Delta_t`, in seconds.

Then a list of fields is provided after `Fields`. These are fields that the model needs, and their names are determined by the model. Below, all fields required by the model (depending on its options) are listed. A generic path (full file name) is then provided (entry `Filename`). In this path, the shortcut '`&f`' refers to a field name. In the previous example, the full path to the temperature is `/u/cergrene/a/ahmed-dm/TestCase-1.0/data/Temperature.bin`. In the specific case of boundary conditions, the shortcut '`&c`' is replaced by x, y and z.

If a few fields are not stored in a file with a generic path, their specific paths can be provided after the entry `Filename`. This is the case for `VerticalDiffusion` in the previous example.

Note that:

1. entries `Fields`, `Filename` and additional paths *must* be at the *end of the section*, and *in this order*;

2. *at least one element* (possibly not a required field) must be provided to `Fields` and at least one element (possibly not a path) to `Filename`; for instance:

```
Fields: ---
Filename: --- # means no generic path.
```

but:

```
Fields:    # Illegal: one element required.
Filename:     # Illegal: one element required.
```

In most sections, `Fields` is used to specify all chemical species involved in the process, e.g.:

```
[deposition]

Date_min: 2001-01-02
Delta_t = 10800.

Fields: O3 NO NO2 H2O2 HCHO PAN HONO SO2 HNO3 OP1 PAA ORA1
Filename: /u/cergrene/A/mallet/2001/data/dep-2005-01-19/&f.bin

ALD   /u/cergrene/A/mallet/2001/data/dep-2005-01-19/ALD-modified.bin
CO    0.002
```

Notice that `CO` is not associated with a path but with a numerical value. This is a feature: a binary file may be replaced with a numerical value. In this case, the field (in the example, CO deposition velocity) is set to a constant value (in every cell and at every time step). This works with any field, including meteorological fields (section `[meteo]`). This feature is often used to set constant boundary conditions.

In `polair3d-data.cfg`, several sections are required. Several sections have to be included only if given options are activated. In the following table, all possible sections are listed, with their entries.

Section	Entries	Comments
`[initial_condition]`	`Fields`, `Filename`	If initial conditions are activated (`With_initial_condition`).
`[boundary_condition]`	`Date_min`, `Delta_t`,`Fields`, `Filename`	If boundary conditions are activated (`With_boundary_condition`).
`[meteo]`	`Date_min`, `Delta_t`, `Fields`, `Filename`	Required fields are: `MeridionalWind` and `ZonalWind` if advection is activated, `VerticalDiffusion` if diffusion is activated, and `Temperature` and `Pressure` in case air density is taken into account.
`[deposition]`	`Date_min`, `Delta_t`, `Fields`, `Filename`	If deposition is activated (`With_deposition`).
`[point_emission]`	`file`	Path to the file which defines the point emissions (described below). If point emissions are activated (`With_point_emissions`).

[surface_emission]	Date_min, Delta_t, Fields, Filename	If surface emissions are activated (With_surface_emission).
[volume_emission]	Date_min, Delta_t, Nz, Fields, Filename	If volume emissions are activated (With_volume_emission). Nz is the number of levels in which pollutants are emitted.
[scavenging]	Fields	If the scavenging model is not set to "none" (Scavenging_model).

The file for point emissions have to contain a section [source] for each point emissions, with the following features:

- its location: Abscissa and Ordinate are given in degrees (or in meters, in case Cartesian coordinates are chosen) and Altitude is the vertical height in meters. Notice that the emission is released in the cell containing the location of the point emission.
- the emitted species is filled after Species. Only one species is possible for each section [source].
- the type Type may be continuous or puff for instantaneous release. The continuous emission is described with entries Rate which corresponds to the quantity averaged on the duration of the release, Date_beg and Date_end which are the beginning and ending dates of the emissions (with format as described in Section 2.2.7). The puff emission is described with entries Quantity and Date.

It may look like this:

```
[source]

Abscissa: 5.2
Ordinate: 48.5
Altitude: 10.

Species: NO

Type: continuous
Rate: 1.
Date_beg: 2001-04-22_00-05
Date_end: 2001-04-22_00-07


[source]

Abscissa: 10.3
Ordinate: 48.
Altitude: 80.

Species: SO2

Type: puff
Quantity: 1.
Date: 2001-04-22_00-05
```

5.5.3 Vertical Levels and Species

Vertical levels are defined in a single data file. They are defined by their interfaces. This means that the file contains `Nz+1` heights, where `Nz` is the number of levels specified in the main configuration file. The concentrations are computed at layers mid-points.

Species are listed in the section `[species]` of a configuration file. In addition, some scavenging models needs extra data:

- The `constant` model requires a section `[scavenging_coefficient]` which contains a threshold of rain to apply scavenging (in $\mathrm{mm\,h^{-1}}$) and the name of the species with its associated scavenging coefficient (in $\mathrm{s^{-1}}$); for instance:

  ```
  [scavenging_coefficient]

  # Scavenging is applied above the following threshold over rain [mm / h].
  Scavenging_rain_threshold: 1.

  # Scavenging coefficient of the species: [s^{-1}]
  NO2 1.e-4       SO2 1.e-4
  ```

  Notice that if the previous lines are replaced by

  ```
  # Scavenging coefficient of the species: [s^{-1}]
  all    1.e-4
  ```

  the same scavenging coefficient will be used for all scavenged species.

- The `belot` model has the following expression $a\,{p_0}^b$ where coefficients a and b have to be provided for every species in a section `[belot]`; for instance:

  ```
  [belot]

  # Coefficients a and b for the Belot parameterization ($a * {p_0}^b$)
  #  where po is the rain intensity  [mm / h].

  # species       a       b
    all           1.e-05  0.8
  ```

- In case the `microphysical` model is used, Henry constants (in $\mathrm{mol\,L^{-1}\,atm^{-1}}$) and gas-phase diffusivities (in $\mathrm{cm^2\,s^{-1}}$) should be provided. Henry constants are listed in section `[henry]`; for instance:

  ```
  [henry]

  # Henry constant: [mol / L / atm]

  O3      1.e-2   NO      2.e-3   NO2     1.e-2   H2O2    1.e5
  HCHO    6.e3    ALD     15.     PAN     3.6     HONO    1.e5
  SO2     1.e5    HNO3    1.e14   OP1     2.4e2   PAA     5.4e2
  ORA1    4.e6    CO      1.e3    N2O5    1.e14
  ```

  Gas-phase diffusivities are provided in the same way in section `[diffusivity]`.

5.6 Polair3DChemistry

Model Polair3DChemistry is configured with three configuration files (`polair3d.cfg`, `polair3d-data.cfg` and `polair3d-saver.cfg`) and two data files (`levels.dat` and `species.dat`). The main configuration file (`polair3d.cfg`) provides the paths to the four other files.

A configuration for Polair3DChemistry is an extension of the configuration for Polair3DTransport. In this section, the description is limited to Polair3DChemistry additional configuration. See Section 5.5 for the rest of the configuration.

5.6.1 Main Configuration File: `polair3d.cfg`

In addition to fields introduced in Section 5.5.1, the following fields are read by Polair3DChemistry:

	`[options]`
`With_chemistry`	Should chemistry occur?
`With_photolysis`	Should photolysis occur?
`With_forced_concentrations`	If activated, the concentrations of a few species are set to values read in files.
`Source_splitting`	If activated, source splitting is used within chemistry integration. Advection and diffusion fluxes are included in the chemistry integration as sources. This slightly increases the memory requirements but is recommended for numerical stability.

5.6.2 Data Description: `polair3d-data.cfg`

In addition to the configuration described in Section 5.5.2, a section `[photolysis_rates]` may be required (if the chemical mechanism includes photolysis reactions). Photolysis rates depend on days, time angle, latitude and altitude. During the time integration, they are linearly interpolated in all cells.

Section	Entries	Comments
`[photolysis_rates]`	`Date_min`	Starting date of photolysis rates.
	`Delta_t`	Time step in days.
	`Ndays`	Number of steps.
	`Time_angle_min`	Starting time angle in hours.
	`Delta_time_angle`	Time angle step in hours.
	`Ntime_angle`	Number of time angles.
	`Latitude_min`	First latitude in degrees.
	`Delta_latitude`	Step along latitude in degrees.
	`Nlatitude`	Number of latitude steps.
	`Altitudes`	List of altitudes in meters at which photolysis rates are provided.
	`Fields, Filename`	Photolysis reaction names and the paths to the files in which photolysis rates are stored.

5.6.3 Vertical Levels and Species

Section 5.5.3 is relevant for Polair3DChemistry, and in particular the file giving the levels is exactly the same. As for species, a section `[molecular_weight]` lists the molecular weights (in $g\,mol^{-1}$) of *all* species. If photolysis reactions are involved, the section `[photolysis_reaction_index]` is required. This section provides all reaction names and their indices in the list of reactions. Below is an example.

```
[photolysis_reaction_index]

NO2      0       O3O1D   1       O3O3P   2       HONO    3
HNO3     4       HNO4    5       NO3NO   6       NO3NO2  7
H2O2     8       HCHOmol 9       HCHOrad 10      ALD     11
MHP      12      HOP     13      PAA     14      KETONE  15
GLYform  16      GLYmol  17      MGLY    18      UDC     19
ORGNIT   20      MACR    21      HKET    22
```

The previous section is quoted from `Polyphemus/driver/species.dat` and is consistent with RACM (as implemented in ChemistryRACM – Section 6.2.1).

5.7 Polair3DAerosol

Polair3DAerosol is configured with three configuration files (`polair3d.cfg`, `polair3d-data.cfg` and `polair3d-saver.cfg`) and two data files (`levels.dat` and `species.dat`). The main configuration file (`polair3d.cfg`) provides the paths to the four other files.

A configuration for Polair3DAerosol is an extension of the configuration for Polair3DChemistry. In this section, the description is limited to Polair3DAerosol additional parameters. See Section 5.6 for the rest of the configuration.

5.7.1 Main Configuration File: `polair3d.cfg`

In addition to fields introduced in Section 5.6.1, the following fields are read by Polair3DChemistry.

	`[domain]`
`Bin_bounds`	The bounds of the diameter classes for aerosol species. Note that the classes are the same for each aerosol species.
	`[options]`
`With_initial_condition_aerosol`	Are initial conditions provided for given aerosol species? If not, initial concentrations are set to zero.
`With_boundary_condition_aerosol`	Are boundary conditions available for given aerosol species?
`With_pH`	Does the aerosol module returns cloud droplet pH?
`Lwc_cloud_threshold`	Liquid water content threshold above which a cloud is diagnosed in the cell.
`Fixed_aerosol_density`	Fixed aerosol density in $kg\,m^{-3}$ used in the model.
`With_deposition_aerosol`	Is dry deposition taken into account for aerosol species?
`Compute_deposition_aerosol`	If set to yes, deposition velocities for aerosol species are computed with land data, otherwise they are read in files. Only needed if dry deposition is taken into account.

With_point_emission_aerosol	Are point emissions provided for aerosol species?
With_surface_emission_aerosol	Are emissions at ground provided for aerosol species?
With_volume_emission_aerosol	Are volume emissions provided for aerosol species?
With_scavenging_aerosol	Is there scavenging for aerosol species?

The bin bounds are presented as follow:

```
Bin_bounds:
# diameter of the particle classes in micrometers.
0.0 0.1 1 1.5 2 5
```

Note that these values are the bounds of the various diameter classes and that therefore there is one more value than there are classes.

5.7.2 Data Description: polair3d-data.cfg

In addition to the sections described in Section 5.6.2, some parameters may be necessary:

Section	Entries	Comments
[initial_condition_aerosol]	Fields, Filename	If initial conditions are activated (With_initial_condition_aerosol).
[boundary_condition_aerosol]	Date_min, Delta_t, Fields, Filename	If boundary conditions are activated (With_boundary_condition_aerosol).
[deposition_velocity_aerosol]	Fields, Filename	If deposition is activated (With_deposition_aerosol) and deposition velocities are not computed (Compute_deposition_aerosol set to no).
[point_emission_aerosol]	file	Path to the file which defines the point emissions. If point emissions are activated (With_point_emissions_aerosol).
[surface_emission_aerosol]	Date_min, Delta_t, Fields, Filename	If surface emissions are activated (With_surface_emission_aerosol).
[volume_emission_aerosol]	Date_min, Delta_t, Nz Fields, Filename	If volume emissions are activated (With_volume_emission_aerosol). Nz is the number of levels in which pollutants are emitted.

5.7.3 Vertical Levels and Species

Section 5.6.3 is relevant for Polair3DAerosol. In addition, there is at least a section added in the file species.dat:

```
[aerosol_species]

PMD    PBC    PNA    PSO4   PNH4  PNO3   PHCL   PARO1
PARO2  PALK1  POLE1  PAPI1  PAPI2 PLIM1  PLIM2  PPOA   PH2O
```

5.8 Polair3DChemistryAssimConc

Polair3DChemistryAssimConc is dedicated for a state space formulation of the underlying dynamical model. The stochastic modeling is implemented for diverse applications such as data

assimilation.

`Polair3DChemistryAssimConc` is configured with three configuration files (`polair3d.cfg`, `polair3d-data.cfg` and `polair3d-saver.cfg`) and two data files (`levels.dat` and `species.dat`). The four files other than the main configuration file (`polair3d.cfg`) are the same as those for `Polair3DChemistry`. The main configuration file is an extension of that of `Polair3DChemistry`.

The additional parameters are:

	`[state]`
`Species`	List of species included in model state vector.
`Levels`	List of vertical levels of model domain included in model state vector.
	`[data_assimilation]`
`Error_covariance_model`	Stochastic model for model and background error covariance. With option set to `Balgovind`, the corresponding error covariance matrix is calculated using Balgovind correlation function; with option set to `diagonal_constant`, the corresponding error covariance matrix is a diagonal matrix of which the diagonal elements are error variances.
`Background_error_variance`	Error variance for background concentrations. The unit for the option value is $\mu g\,m^{-3}$.
`Balgovind_scale_background`	Balgovind scale for background error covariance. The model grid interval is chosen to be the unit for option values.
`Model_error_variance`	Error variance for model simulations (in $\mu g\,m^{-3}$).
`Balgovind_scale_model`	Balgovind scale for model error covariance. The model grid interval is chosen to be the unit for option values.
	`[observation_management]`
`Configuration_file`	Choose between observation.cfg (to use observations) and observation-sim.cfg (to use simulated observations).

The data file is the same as in Section 5.6.2, the species and levels files are the same as those presented in Section 5.6.3.

5.9 CastorTransport

5.9.1 Main Configuration File: `castor.cfg`

Model `CastorTransport` is based on IPSL model Chimere. Its option are provided in a configuration file:

	`[domain]`
`Date_min`	Starting date in any legal format (see Section 2.2.7). The date can therefore include seconds.
`Delta_t`	Time step in seconds.
`Nt`	Number of iterations of the simulation (integer).
`x_min`	Abscissa of the center of the lower-left cell. Provide a longitude (in degrees) or, in case Cartesian coordinates are chosen, an abscissa in meters.

Delta_x	Step length along x, in degrees (longitude) or in meters (for Cartesian coordinates).
Nx	Number of cells along x (integer).
y_min	Ordinate of the center of the lower-left cell. Provide a latitude (in degrees) or, in case Cartesian coordinates are chosen, an ordinate in meters.
Delta_y	Step length along y, in degrees (latitude) or in meters (for Cartesian coordinates).
Ny	Number of cells along y (integer).
Nz	Number of vertical levels (integer).
Vertical_levels	Path to the file that defines vertical levels interfaces. This field is read but is not used.
Species	Path to the file that defines involved species and their chemical properties.
	[options]
With_transport	Is transport taken into account?
With_initial_condition	Are initial conditions used?
Interpolated_initial_condition	If set to yes, initial conditions are interpolated from boundary conditions, otherwise they are read in binary files.
With_boundary_condition	Are boundary conditions provided?
With_deposition	Is deposition taken into account?
With_volume_emission	Are volume emissions taken into account?
	[data]
Data_description	Path to the configuration file that describes input data.

5.9.2 Data Description: castor-data.cfg

The data description is very similar to that of Polair3DTransport (see Section 5.5.1), except that the data can be different.

Section	Entries	Comments
[initial_condition]	Fields, Filename	If initial conditions are activated (With_initial_condition) and not interpolated (Interpolated_initial_condition set to no).
[boundary_condition]	Fields, Filename	If boundary conditions are activated (With_boundary_condition).
[meteo]	Date_min, Delta_t, Fields, Filename	Required fields are: Temperature, Pressure, Altitude, AirDensity, MeridionalWind, ZonalWind and VerticalDiffusion.
[deposition]	Date_min, Delta_t, Fields, Filename	If deposition is activated (With_deposition).
[volume_emission]	Date_min, Delta_t, Nz, Fields, Filename	If volume emissions are activated (With_volume_emission). Nz is the number of levels in which pollutants are emitted.

5.9.3 Vertical Levels and Species

A file containing vertical levels similar to the one for "Polair" models is read but is not useful. Give any such file.

Species file has two sections:

- `[species]` which contains all species managed by the simulation.
- `[species_ppm]` which contains all species for which an upwind scheme is not used.

Chapter 6

Modules

6.1 Transport modules

6.1.1 AdvectionDST3

Module `AdvectionDST3` is the transport module associated to advection for `Polair3D`. It is based on a third-order "direct space-time" scheme with a Koren-Sweby flux limiter. The data needed are the wind components and boundary conditions if they are available.

Please note that Courant-Friedrichs-Lewy (CFL) condition is not verified and that the user should choose the mesh dimensions and the time-step of simulations very carefully.

6.1.2 DiffusionROS2

Module `DiffusionROS2` is the transport module associated to diffusion for `Polair3D`. It is based on a second-order Rosenbrock method. Fortran routines are used to perform all numerical computations.

6.1.3 TransportPPM

Module `TransportPPM` is the numerical solver for transport used in Castor model. It uses piecewise parabolic method (PPM) for advection but can also use an upwind scheme for some species.

In the species file associated with castor there are two sections: `[species]` and `[ppm_species]`. For all species in `[species]` but not in `[ppm_species]` an upwind scheme will be used.

6.2 Chemistry Modules

6.2.1 ChemistryRACM

Module `ChemistryRACM` is the most common photochemical module used with Polair3D. It implements RACM (Stockwell et al. [1997]) and uses a second-order Rosenbrock method for time integration. Computations are performed by Fortran routines (automatically generated by the chemical preprocessor SPACK) and a C++ program is used as a frame to launch all these calculations.

It only deals with gaseous species and manages 72 species, 237 reactions (including 23 photolysis reactions).

6.2.2 ChemistryRACM_SIREAM

Remark Before using this module, please read the file `README-SIREAM` provided in `driver`.

To use this module, *sources* for ISORROPIA (Nenes et al. [1998]) are necessary. You can obtain them from its home page `http://nenes.eas.gatech.edu/ISORROPIA/`.

Another step before using ChemistryRACM_SIREAM is to modify slightly the file `Polair3DChemistry.cxx` in `models`:

- l 414 and 415: comment out

```
if (this->option_process["with_chemistry"])
  Chemistry_.Init(*this);
```

- l 601: comment out

```
Chemistry_.Forward(*this);
```

And finally compile the file `polair3d-siream.cpp` using the makefile `makefile.siream` provided. A specific makefile has been provided because ChemistryRACM_SIREAM redefines some Fortran routines defined by ChemistryRACM.

ChemistryRACM_SIREAM This chemistry module is used for gas and aerosol species for general purposes as air quality modeling and risk assessment. The gas chemistry is solved with the RACM (Stockwell et al. [1997]) mechanism and the aerosol dynamics by the SIREAM model (Debry et al. [2006]). When a cloud is diagnosed in one cell of the domain, then instantaneous aerosol activation is assumed and the SIREAM model is replaced by the VSRM cloud chemistry model (Fahey and Pandis [2003]).

The number of aerosol bins is directly inferred from the number of bounds provided by the `Bin_bounds` option in main configuration file (`polair3d.cfg`). Further options are required in this configuration file.

	`[options]`
`With_pH`	Does the aerosol module returns cloud droplet pH?
`Scavenging_model`	Which below cloud scavenging model is used?
`Lwc_cloud_threshold`	Liquid water content threshold for clouds.
`With_coagulation`	Is coagulation taken into account?
`With_condensation`	Is condensation taken into account?
`With_nucleation`	Is nucleation taken into account?
`Fixed_aerosol_density`	Fixed aerosol density in $\mathrm{kg\,m^{-3}}$ used in the module
`With_cloud_chemistry`	Is cloud chemistry taken into account?
`With_in_cloud_scavenging`	Is in-cloud scavenging taken into account?
`With_heterogeneous_reactions`	Are heterogeneous reactions taken into account?
`With_kelvin_effect`	Is Kelvin effect taken into account?
`Dynamic_condensation_solver`	Which solver is used for dynamic condensation?
`Fixed_cutting_diameter`	Fixed cutting diameter in µm.
`Sulfate_computation`	Which method is used to solve sulfate condensation? Choices are `equilibrium` or `dynamic`.
`Redistribution_method`	Which redistribution method is used?
`Nucleation_model`	Which nucleation model is used?
`With_fixed_density`	Is aerosol density fixed in the module?
`Wet_diameter_estimation`	Which method is used to compute aerosol wet diameters?

The liquid water content threshold is the amount of liquid water in the air above which a cloud is diagnosed in the cell.

This chemistry module returns the cloud droplet pH, this means that `With_pH` can be set to yes, and that `microphysical-pH` scavenging model can be used. Otherwise choosing the `microphysical-pH` scavenging model may result in crash or errors.

Note that options `With_pH`, `Lwc_cloud_threshold` and `Fixed_aerosol_density` are used by both model and module. That is to say the fixed aerosol density is the same in the model as in the module.

The fixed cutting diameter has to be given as an aerosol diameter in µm. Aerosol bins below that diameter are assumed at equilibrium, and those above that diameter are not considered at equilibrium. The criteria is the comparison between the fixed cutting diameter and the bin bounds. The aerosol bin whose bounds are surrounding the fixed cutting diameter is included in the equilibrium bins.

Dynamic condensation is intended for aerosol bins which are not at equilibrium, and therefore time resolved mass transfer has to be computed for them. The solver for dynamic condensation may be set to either `etr` or `ros2` or `ebi`. The `etr` solver is an Explicit Trapezoidal Rule second order algorithm, the `ros2` solver is the Rosenbrock implicit second order scheme (Rosenbrock [1963]), and `ebi` is an Euler Backward Iterative scheme. Each of these solvers usually needs some numerical parameters, these are gathered in the Fortran include file `paraero.inc`.

Option `With_kelvin_effect` only affects dynamic bins.

Among aerosol species, sulfate condensation may have a different treatment. If `Sulfate_computation` is set to `equilibrium` then its treatment is equivalent to other species for both equilibrium and dynamic bins. But if it is set to `dynamic` then sulfate condensation is time resolved for all bins, using an analytic solution of mass transfer equations. This method is implemented in the `sulfdyn.f` Fortran routine.

As dynamic condensation is solved with a Lagrangian scheme, a redistribution process over the fixed aerosol size grid has to be performed at the end of condensation. Two methods are possible: `number-conserving` or `interpolation`. The former conserves the relationship between mass and number concentration in each bin, the latter relaxes this relationship.

Available nucleation models are either `binary` nucleation H_2SO_4–H_2O (Vehkamäki et al. [2002]) or `ternary` nucleation H_2SO_4–H_2O–NH_3 (Arstila et al. [1999]).

In the aerosol module, the aerosol density can be either fixed or recomputed at run time according to option `With_fixed_density`. If set to yes the aerosol density will always be equal to the fixed aerosol density mentioned above, if set to no the module will recompute one density for each aerosol bins according to their chemical compositions given by the thermodynamic model.

Two parameterizations are available to compute wet diameters depending on the option `Wet_diameter_estimation`. If set to `Isorropia` the aerosol liquid water content computed by the thermodynamic model, for instance ISORROPIA, is used. If set to `Gerber`, a simpler but faster method, the Gerber formula, is used.

Note that when `Gerber` option is used, the aerosol density is fixed for all aerosol processes except condensation even if option `With_fixed_density` is set to no. In other words if run time computation of density is chosen, it will only affect condensation. Indeed when using the Gerber formula for fastness purpose there is little interest in recomputing density. Then the fixed density is that specified with `Fixed_aerosol_density` option.

6.2.3 ChemistryRADM

Module `ChemistryRADM` is quite similar to `ChemistryRACM`. RACM has actually been derived from RADM.

RADM manages 61 species, 157 reactions involving those species and 21 photolysis reactions.

6.2.4 ChemistryCastor

Module `ChemistryCastor` is the default chemical module for `Castor`. It involves 44 species and 118 reactions. It is based on several data files which must be provided: `Reaction_file`, `Stoichiometry_file`, `Photolysis_file` and `Rate_file`.

6.2.5 Decay

This chemistry module is used for species (gaseous or particulate) which have a radioactive or biological decay, that is to say a natural decrease in their concentrations over time. This decay requires two more options in the configuration file (`polair3d.cfg`).

[options]	
`With_time_dependence`	If set to yes, the value of the half-life time for each species depend on the time of the day (see below).
`With_filiation_matrix`	If set to yes, decay and filiation are represented by a matrix (see below).

Note that `With_time_dependence` and `With_filiation_matrix` cannot be both set to yes at the same time.

Use of One Value of Decay The first possibility is that each species has a half-life time which is given in `species.dat`. In that case `With_time_dependence` and `With_filiation_matrix` are both set to no. The variation of concentration due to decay only is described in equation (6.1) where $T_{1/2}$ is the species half-life time in days and t_0 is a reference time. If a species has no decay, its half-life time is set to 0, and this is interpreted by `Decay` as the fact that concentration does not vary due to decay.

$$C(t) = C(t_0) \exp\left(-\frac{(t - t_0)\ln 2}{T_{1/2}}\right) \tag{6.1}$$

The parameters needed are provided in `species.dat` as follow.

```
[species]

Sp1 Sp2 Sp3 Sp4

[aerosol_species]

Aer1 Aer2

[half_life]

# Half-lives in days, put 0 for species without decay.
Sp1 300
Sp2 216
Sp3 0
Sp4 41
```

```
[half_life_aerosol]

# Half-lives in days, put 0 for species without decay.
Aer1   250
Aer2   120
```

Use of Two Values of Decay Another option is that each species has two values of $T_{1/2}$, one for the day and one for the night. This is in particular the case for species which have a biological effect. As before, for a species without decay, both half-life times are set to 0. The equation involved is very similar to equation (6.1), except that the value of $T_{1/2}$ can vary. In that case `With_time_dependence` is set to yes and `With_filiation_matrix` to no.

The parameters needed are provided in `species.dat`.

```
[species]

Sp1 Sp2 Sp3 Sp4

[aerosol_species]

Aer1 Aer2

[half_life_time]

# Half-lives in days, put 0 for species without decay.
# First value for day, second for night.

Sp1 300 500
Sp2 216 300
Sp3 0 0
Sp4 41 72

[half_life_time_aerosol]

# Half-lives in days, put 0 for species without decay.
# First value for day, second for night.
Aer1: 250 350
Aer2: 120 180
```

`Decay` tests whether it is day or night and chooses the value of half-life time to use.

Use of a Filiation Matrix The last solution is that a single matrix (called filiation matrix) is specified for all gaseous species (and one for all aerosol species), which takes into account both decay and the fact that a species can react to form other species. As a result, the evolution of the concentration due to chemistry only is described in equation (6.2). In that case `With_time_dependence` is set to no and `With_filiation_matrix` to yes.

$$C^{n+1}(x,y,z) = AC^{n}(x,y,z) \tag{6.2}$$

where A is the $s \times s$ *filiation matrix* and $C^n(x,y,z) = \begin{pmatrix} c_0^n(x,y,z) \\ \dots \\ c_i^n(x,y,z) \\ \dots \\ c_{s-1}^n(x,y,z) \end{pmatrix}$ with $c_i^n(x,y,z)$ the concentration of species i at time-step n in point of coordinate (x,y,z) and s the number of species involved.

The parameters are specified as follows, in `species.dat`

```
[species]

Sp1 Sp2 Sp3 Sp4

[aerosol_species]

Aer1 Aer2

[filiation_matrix]
File: example/decay/matrix.dat

[filiation_matrix_aerosol]
File: example/decay/matrix_aer.dat
```

The $s \times s$ filiation matrix is specified in file matrix.dat as below :

```
0.7 0.05 0 0.1
0 0.8 0.1 0.05
0.1 0.1 0.6 0.1
0.15 0 0.1 0.7
```

The matrix for aerosol species is very similar to the one for gaseous species.

Chapter 7

Postprocessing

7.1 Visualizing Results

7.1.1 Configuration File: `disp.cfg`

Once you have checked that your binary files seem to be all right (see Section 2.5.6), you may want to visualize the results. The first step to do that using Matplotlib[†1] is to create a configuration file - usually named "disp.cfg" - which contains the following information:

`[input]`	
`Nt`	Number of time steps for which the concentrations are saved.
`Nx`	Space steps in the x direction.
`Ny`	Space steps in the y direction.
`Nz`	Number of vertical layers on which concentrations are saved.
`file`	Binary file containing the results to be visualized (relative or absolute path).

Here is an example of such a configuration file:

```
[input]

Nt = 121
x_min    = -10.0  Delta_x = 0.5  Nx = 67
y_min    = 35     Delta_y = 0.5  Ny = 46
Nz = 8

file: /u/cergrene/a/ahmed-dm/Polyphemus-RC/driver/results/O3.bin
```

An easy way to do that is to copy the section `[domain]` of the configuration file used for the simulation in this file. But the number of time steps and vertical layers might be different from those used for the simulation, for it depends on what has been specified in the saver configuration file.

7.1.2 Visualizing Results

The quicker way to visualize the results is to use the interactive python interpreter IPython (launched with the command `ipython`). However, you can also write your commands into a

[†1] http://matplotlib.sourceforge.net/

python script that you will launch afterwards with the command `python script.py`. In any case, you must first check that the program `extract_configuration` (see Section 1.3) has been compiled before you follow the steps below.

First you need to make sure that Python will look in `include/atmopy` for unknown modules. Therefore, to use it, it is necessary to put it in the `$PYTHONPATH`. For example, for bash users:

```
export PYTHONPATH=~/usr/lib/python
```

Using a Background Map

In the case of continental simulations, follow these steps to visualize your results with a background map corresponding to your simulation domain. That is irrelevant in the case of regional or local simulations, especially if you are using Cartesian coordinates instead of longitude/latitude.

1. The first step is to import the modules that are needed:

   ```
   import atmopy
   from atmopy.display import *
   ```

2. Then, import the data from the configuration file:

   ```
   m, d = getmd('disp.cfg')
   ```

   In that step, you have created an array named 'd' (but you can name it otherwise) which contains your results. It is a 4D-array of shape $N_t \times N_z \times N_y \times N_x$ given in the configuration file. You can access a concentration at time t, level z, point (x,y) with the command `d[t, z, y, x]`. You can also verify its shape with the command `d.shape`.

3. Display the concentration map at time step t and vertical level z:

   ```
   disp(m, d[t, z])
   ```

Figure 7.1 gives an example of output figure with the command `disp(m, d[t, z])`. The simulation domain corresponds to Europe, so that is the background map.

You can afterwards save the figures in any format you wish (*.png, *.eps, ...).

If you want to display results for several species, you do not have to create the background map each time because you will use the same for all species. In that case, for all species but the first, create only a data with function `getd`. This is similar to what is shown below.

Without a Background Map

The following steps allow you to visualize your results without a background map. This is especially required in the case of local simulations, so the example given here has been made with Gaussian models.

1. The first step is to import the modules that are needed:

   ```
   import atmopy
   from atmopy.display import *
   ```

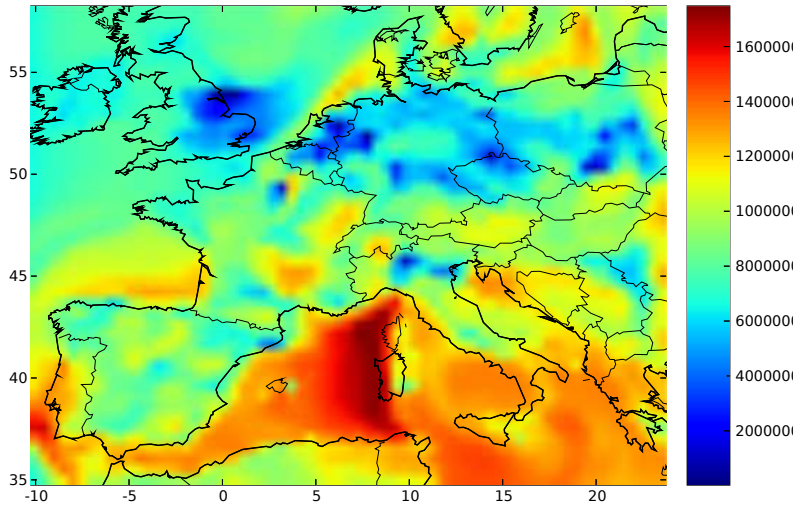


Figure 7.1: Concentration map obtained with the command `disp`.

2. Then, import the data from the configuration file:

   ```
   d = getd('disp.cfg')
   ```

   In that step, you have created an array named 'd' (but you can name it otherwise) which contains your results. It is a 4D-array of shape $N_t \times N_z \times N_y \times N_x$ given in the configuration file. You can access a concentration at time t, level z, point (x,y) with the command `d[t, z, y, x]`. You can also verify its shape with the command `d.shape`.

3. Display the concentration at time step t and vertical level z:

   ```
   contourf(d[t, z])
   ```

4. Add a colorbar. You can specify the type of notation you want in the colorbar:

   - `colorbar('%n.mf')` to have numbers in decimal format with n significant figures before the dot and m significant figures after.
   - `colorbar('%n.me')` to have numbers in scientific notation with n significant figures before the dot and m significant figures after.
   -

Figure 7.2 gives an example of concentration map.

Note that: In that case, the information necessary is only N_t, N_z, N_y and N_x, and the filename. You don't need to use a configuration file to give these parameters, you can also modify the call to function `getd` :

```
d = getd(filename='O3.bin', Nt = 24, Nz = 1, Ny = 19, Nx = 13)
```

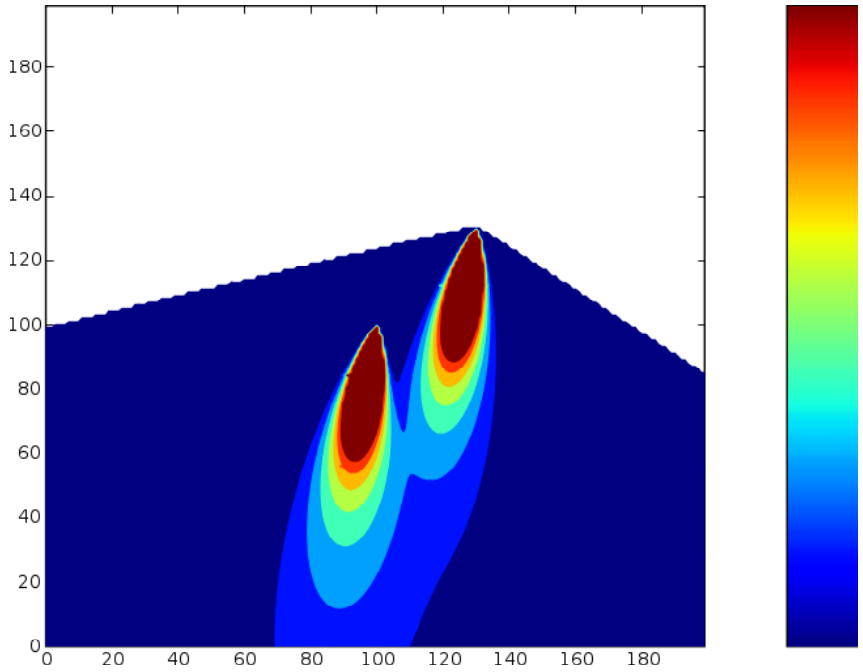


Figure 7.2: Concentration map obtained with the command `contourf`.

7.2 Aerosol Postprocessing

7.2.1 Configuration File

The configuration file `simulation_aerosol.cfg` is the same as `simulation.cfg` described previously, where aerosol parameters are added:

[input]	
`Nbins`	Number of size bins.
`computed`	If yes, the bin bounds are computed using a logarithmic law. If no, they are given in a file.
`Dmin, Dmax`	If bin bounds are computed, the minimum and the maximum diameters.
`file_bounds`	If bin bounds are given in a file, the name of the file.
`bin_index_shift`	Number of the first bin (typically 0 or 1).
`primary`	Names of the primary species in the model.
`inorganics`	Names of the inorganic species in the model.
`organics`	Names of the organic species in the model.
`primary_names`	Real names of the primary species (to be displayed).
`inorganics_names`	Real names of the inorganic species (to be displayed).
`output_species`	Aggregated data in output (PM_{10}, $PM_{2.5}$, total mass for each chemical component, total mass and number in each bin).
`with_organics`	If yes, total masses will take into account organic species.
`graph_type`	Graphs that will be displayed when launching `graph_aerosol.py` (chemical composition, mass and number distribution, time series).
`graphs_at_station`	If yes, the graphs will be displayed for the simulation at a given station. If no, graphs will be an average over the domain defined by `i_range` and `j_range`.

i_range	First and last indices in x direction for the considered domain.
j_range	First and last indices in y direction for the considered domain.
log_plot	If yes, the mass and number distributions will be displayed with a log scale for diameters.
directory_list	List of directories where outputs are, the aggregated data will be written in a file in the same directory as the output.

The file simulation_aerosol.cfg is used by scripts init_aerosol.py and graph_aerosol.py.

7.2.2 Script init_aerosol.py

The outputs of the model for aerosols will be several files: <species>_<number>.bin where <species> is an aerosol chemical component (in [aerosol_species], see Section 5.5.3) and <number> is the index of the size bin. But often, measurements are aggregated data:

- PM_{10} and $PM_{2.5}$ are the mass of aerosol with a diameter smaller than 10 µm and 2.5 µm respectively,
- Total mass of one chemical component.

One can also be interested by the number of particles in each size bin (granulometry), or by the mass distribution along the size bins. This will be done by the script graph_aerosol.py, but before you have to launch init_aerosol.py by the command:

```
python init_aerosol.py simulation_aerosol.cfg
```

Then you can launch disp.py and evaluation.py with species such as PM10, PM2.5, PNA (total mass for sodium), etc.

7.2.3 Script graph_aerosol.py

You can launch graph_aerosol.py by the command:

```
python graph_aerosol.py simulation_aerosol.cfg}
```

Then each desired graphs (specified in graph_type section of the configuration file) will be displayed in a different window.

Appendix A

Polyphemus Eulerian Test-Case

The test case is available on Polyphemus site[†1]. In order to use the test-case, you should download:

- The meteorological data file `MM5-2004-08-09.tar.bz2`. The file is not included in the test-case so that it can be used for various applications and has not to be downloaded each time.
- The archive `TestCase.tar.bz2`.

Note that you should have Polyphemus installed and working in order to use the test-case.

A.1 Preparing the Test-Case

The first step is to extract the archive `TestCase.tar.bz2`

```
tar -xjvf TestCase.tar.bz2
```

The directory `TestCase` that will be created is divided in four subdirectories:

- `data`, which contains all precomputed data.
- `raw_data`, which contains all data used for preprocessing. After preprocessing, the results are stored in `data` to be used directly during the simulation.
- `config`, where configuration files are provided.
- `results`, where the results of the simulation are stored.

In addition a file `version` is included to indicate for which version of Polyphemus the test-case is designed, and which versions of the libraries are needed.

`MM5-2004-08-09` should be extracted and then placed in `raw_data`.

```
tar -xjvf MM5-2004-08-09.tar.bz2
mv MM5-2004-08-09 TestCase/raw_data/MM5/
```

Now you have all data necessary to perform preprocessing for the ground and for meteorological data. All other data (emissions, deposition velocities ...) are provided and ready-to-use.

[†1] `http://www.enpc.fr/cerea/polyphemus/`

A.2 Modifying the General Configuration File

The file `general.cfg` is used by all preprocessing programs and as such must be the first file you modify when performing preprocessing. Make sure to modify and use the file provided in the directory `TestCase/config`. Here is a copy of this file:

```
[general]

Home: /u/cergrene/a/ahmed-dm
Path_to_test_case: <Home>/TestCase-1.0
Path_to_polyphemus: <Home>/Polyphemus-1.0

Directory_raw_data: <Path_to_test_case>/raw_data
Directory_computed_fields: <Path_to_test_case>/data
Directory_ground_data: <Directory_computed_fields>/ground
Programs: <Path_to_polyphemus>/preprocessing


[domain]

Date: 20040809
t_min = 0.0     Delta_t = 1.0   Nt = 24
x_min = -10.0   Delta_x = 0.5   Nx = 65
y_min = 40.5    Delta_y = 0.5   Ny = 33
Nz = 5
Vertical_levels: <Programs>/levels.dat
```

Replace `Home` by the path to your home directory, `Path_to_test_case` by the path to `TestCase` and `Path_to_polyphemus` by the path to `Polyphemus`. Other paths needed for the simulation depend on these ones so modifying them should be sufficient. The domain is defined for a simulation over Europe. Make sure that the date is 20040809 (date for which meteorological raw data is provided).

It is advised to put both `TestCase` and `Polyphemus` in your home directory, as this is what will be used below.

A.3 Computing Ground Data

Ground data are not necessary to perform the simulation but they are needed to compute the vertical diffusion using Troen and Mahrt parameterization. If you wish to use Louis parameterization, this step is not necessary and you can go to Section A.4.

A.3.1 Land Use Cover

Compile and execute `luc-usgs` (from your `Polyphemus` directory):

```
cd Polyphemus/preprocessing/ground
make luc-usgs
./luc-usgs ~/TestCase/config/luc-usgs.cfg  ~/TestCase/config/general.cfg
```

The output on screen will be:

```
Reading configuration files... done.
Memory allocation for data fields... done.

Reading LUC data... done.
Building LUC data on output grid... done.

Writing output data... done.
```

A.3.2 Roughness

The preprocessing program `roughness` needs as input data the results of `luc-usgs`.

The file `roughness.cfg` in `Polyphemus/preprocessing/ground` should be ready to use (just check that the markup `LUC_origin` is set to "usgs"). Then compile and execute `roughness`.

```
make roughness
./roughness roughness.cfg  ~/TestCase/config/general.cfg
```

The output on screen will be:

```
Reading configuration files... done.
Reading roughness data... done.
Writing roughness binary ... done.
```

A.4 Computing Meteorological Data

No modification to configuration file `MM5-meteo.cfg` should be necessary but make sure to use the version of this file included in directory `TestCase` and not in directory `Polyphemus`.

You can open the file and check that `Database_MM5-meteo` is the path to the file `MM5-2004-08-09`, where the date is represented by `&D`. For details about the other options available in the configuration file, see Section 3.4.5.

Then compile MM5-meteo:

```
cd ../meteo
make MM5-meteo
```

and execute it:

```
./MM5-meteo ~/TestCase/config/MM5-meteo.cfg ~/TestCase/config/general.cfg 20040809
```

The output on screen will be:

```
Reading configuration files... done.
Memory allocation for grids... done.
Memory allocation for output data fields... done.
Conversion from sigma levels to heights... done.
Converting from latlon to MM5 indices... done.
Applying transformation to read fields... done.
Computing pressure... done.
Computing surface pressure... done.
Interpolations... done.
Computing Richardson number... done.
Computing attenuation...
```

```
  + Computing relative humidity and critical relative humidity... done.
  + Computing cloud profile... done.
  + Computing attenuation... done.
Linear interpolations...
  + Attenuation
  + SpecificHumidity
  + Liquid Water content
  + CloudHeight
  + SurfaceTemperature
  + SkinTemperature
  + SoilWater
  + SensibleHeat
  + Evaporation
  + SolarRadiation
  + Rain
  + FrictionModule
  + BoundaryHeight
 done.
Computing Kz... done.
Computing PAR... done.
Writing data... done.
```

If you want to compute vertical diffusion using Troen and Mahrt parameterization, compile and execute `Kz_TM`.

```
make Kz_TM
./Kz_TM ~/TestCase/config/MM5-meteo.cfg  ~/TestCase/config/general.cfg 20040809
```

The output on screen will be:

```
Reading configuration files... done.
Memory allocation for data fields... done.

Extracting fields... done.

Computing Kz... done.
Writing output files... done.
```

A.5 Launching the Simulation

A.5.1 Modifying the Configuration File

You should check and modify `polair3d.cfg` if necessary. You have to check the paths (in particular check that the data and saver files are `config/polair3d-data.cfg` and `config/polair3d-saver.cfg`) and to make sure that the date for the simulation is 20040809 (date for which the meteorological data have been computed).

A.5.2 Modifying the Data File

Check `config/polair3d-data.cfg`. If you decided to use Louis parameterization for vertical diffusion, modify the file associated to `VerticalDiffusion` in the section `[meteo]`.

As before, check the paths and dates. In particular, if the dates in any section (except for `[photolysis]`, see below) are not right, you can have an error message.

```
ERROR!
An input/output operation failed in FormatBinary<T>::
Read(ifstream& FileStream, Array<TA, N>& A).
   Unable to read 42900 byte(s). The input stream is empty.
```

Indeed, input data can be computed for several days, so the program will discard the data for the days between `Date_min` in a section of `polair3d-data` and `Date_min` for the simulation. Here, as the data has been computed for one day only, it would be as if the data files were empty, hence this error.

Remark In the case of photolysis, data are provided for a whole year and `Date_min` must be `2004-01-01_12`.

A.5.3 Modifying Saver File

The file `polair3d-saver.cfg` should be ready to use. You can modify the species to save (you are advised against saving concentrations for all species). You can choose to save instantaneous concentrations or concentrations averaged over `Interval_length` by setting `Averaged` to no or yes respectively.

A.5.4 Simulation

Compile the driver.

```
cd ../../Polyphemus/driver
make polair3d
```

Launch the simulation from `TestCase`:

```
cd ../../TestCase/
../Polyphemus/driver/polair3d config/polair3d.cfg
```

A.6 Visualizing Results

A.6.1 Modifying Configuration File

Modify `results/disp.cfg` if necessary (in particular if you have modified `polair3d-saver.cfg`).

```
[input]

# Number of time steps for which concentrations are saved.
Nt = 22
# Domain description for x and y.
x_min    = -10.0     Delta_x = 0.5     Nx = 65
y_min    = 40.5      Delta_y = 0.5     Ny = 33
# Number of levels for which concentration are saved.
Nz = 1

file: O3.bin
```

A.6.2 Using IPython

For details see Section 7.1.2. Remember that the directory `atmopy` should be in your `$PYTHONPATH`. Launch IPython and then type in command line (comments starting with "#"have been added to explain the meaning of each line):

```
from atmopy.display import *    # Import to the interactive session all
                                # functions from the module 'display'
                                # of 'atmopy'
m = getm('disp.cfg')            # Create the map.
d = getd('disp.cfg')            # Create a data with the results.
dispcf(m, d[7,0])               # Display the data for the 8th time step
                                # and the first vertical level (remember
                                # that indices start at 0).
```

The image obtained is Figure A.1.

You can create other data if you like to visualize concentrations for other species. In that case, the map has already been created and less information is needed to create the data. In particular it is not necessary to provide a file `disp.cfg`:

```
d2 = getd(filename = 'NO.bin', Nt = 22, Nz = 1, Ny = 33, Nx = 65)
disp(m, d2[7,0])
```

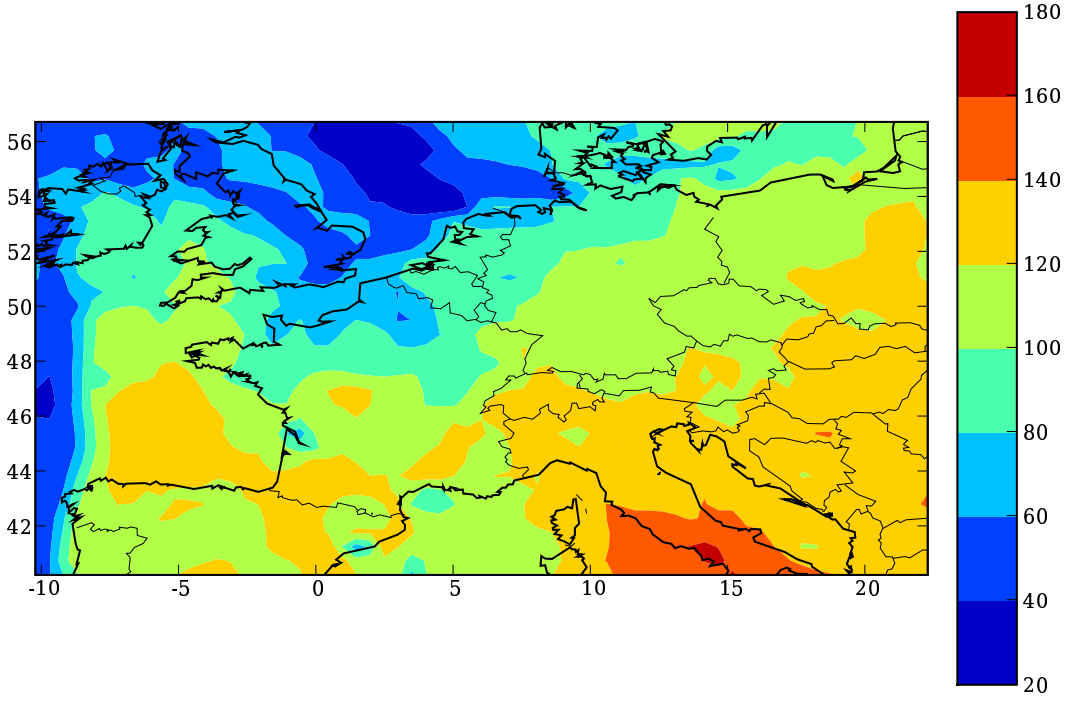


Figure A.1: Figure obtained using IPython and AtmoPy (unit is $\mu g\,m^{-3}$)

Appendix B

Polyphemus Gaussian Test-Case

This document explains how to proceed to perform simulations using the test case for Gaussian models provided with Polyphemus.

When the archive `TestCase-1.0-Gaussian.tar.bz2` is extracted a directory `TestCase-1.0-Gaussian/` is created. It is referred to below as `TestCase`.

```
tar -xjvf TestCase-1.0-Gaussian.tar.bz2
```

The subdirectory `config/` holds all configuration files necessary and the subdirectory `results/` is meant to store the results of simulations. It is divided in three subdirectories (one for each possible simulation) : `puff_line/` for the Gaussian puff model and a gaseous line source, `puff_aer/` for the puff model with point sources of gaseous and aerosol species, and `plume/` for the Gaussian plume model with gaseous species only. In each of those subdirectory a python program which allows to visualize some results easily can be found.

To launch the test cases, you do not need to modify the configuration files. You just have to make sure to replace `Polyphemus/` and `TestCase/` by your path to the last version of Polyphemus and the Gaussian test case respectively.

B.1 Preprocessing

Prior to use Gaussian models, you need to compute scavenging coefficients and deposition velocities for the various species. This is achieved by using `gaussian-deposition_aer`.

First compile it :

```
cd ~/Polyphemus/preprocessing/dep/
make gaussian-deposition_aer
```

Then run it from the test case directory:

```
cd ~/TestCase/
~/Polyphemus/preprocessing/dep/gaussian-deposition_aer
                        config/gaussian-deposition_aer.cfg
```

The output on screen will be :

```
Reading configuration file... done.
Reading meteorological data... done.
```

```
Reading species... done.
Reading diameter... done.
Computation of the scavenging coefficients... done.
Computation of the deposition velocities..done.
Writing data... done.
```

The file `gaussian-meteo_aer.dat` has been created in the directory `TestCase/config/`. It will be used for all simulations.

Note that if your simulation only involves gaseous species, you can use the preprocessing program `gaussian-deposition`. Here we use `gaussian-deposition_aer` because its output can be used for simulations with or without aerosol species.

B.2 Discretization

This step is only necessary for the simulation with a line source. Its aim is to discretize this source into a series of puffs. To do so, compile the preprocessing program `discretization`:

```
cd ~/Polyphemus/preprocessing/emissions/
make discretization
```

Then run it from the test case directory:

```
cd ~/TestCase/
~/Polyphemus/preprocessing/emissions/discretization
                                config/discretization.cfg
```

The output on screen will be:

```
Reading configuration file... done.
Reading trajectory data... done.
Length of the trajectory: 48.0278
Number of points on the trajectory: 26
Writing source data... done.
```

The file `puff-source-discretized.dat` has been created in the directory `TestCase/config`. It contains a series of puffs representing the discretized line source.

B.3 Simulations

B.3.1 Plume

This simulation uses the program `plume`, which is the program for the Gaussian plume model. It uses the following data:

- Gaseous species : Caesium, Iodine.
- Sources : 2 point sources for Iodine, one point source for Caesium.
- Meteorological situations : 4 situations, rotating wind with an increasing speed (0.1m/s, 2m/s, 5m/s et 10m/s).
- Urban environment.

The simulation uses the following files :

- `plume.cfg` gives the simulation domain, the options and the paths to the other files.
- `gaussian-levels.dat` gives the vertical levels.
- `gaussian-species_aer.dat` gives all meteorological data and scavenging and deposition coefficients. It was created during preprocessing (see Section B.1).
- `plume-source.dat` contains all the data on stationary sources.
- `plume-saver.cfg` contains the options and paths to save the results.

Compile the program plume :

```
cd ~/Polyphemus/driver/
make plume
```

Then execute it from `TestCase/` :

```
cd ~/TestCase/
~/Polyphemus/driver/plume config/plume.cfg
```

The output on screen will be :

```
        Temperature     Wind angle      Wind velocity   Stability
Case #0
        15              -100            0.5             D
Case #1
        10              -5              2               D
Case #2
        10              20              5               D
Case #3
        10              60              10              D
```

Results are stored in `results/plume/`.

B.3.2 Puff with Aerosol Species

The simulation uses `puff_aer`, which is the program for puffs with aerosol species, and the following data:

- Gaseous species : Caesium, Iodine.
- Aerosol species : aer1, aer2.
- Sources : 1 point source per species.
- Meteorological situations : 4 situations, rotating wind with an increasing speed (0.1m/s, 2m/s, 5m/s et 10m/s).
- Urban environment.

The simulation uses the following files:

- `puff_aer.cfg` gives the simulation domain, options and the paths to the other files.

- `gaussian-levels.dat` gives the vertical levels.
- `gaussian-species_aer.dat` gives all meteorological data and data on scavenging and deposition. It was created during preprocessing (see Section B.1).
- `puff-source_aer.dat` contains all the data on gaseous and aerosol sources.
- `puff-saver_aer.cfg` contains the options and paths to save the results.

Compile the program `puff_aer`:

```
cd ~/Polyphemus/driver/
make puff_aer
```

Then execute it from `TestCase/`:

```
cd ~/TestCase/
~/Polyphemus/driver/puff_aer config/puff_aer.cfg
```

Results are stored in `results/puff_aer/`.

B.3.3 Puff with Line Source

The simulation uses `puff`, which is the program for puffs with gaseous species only, and the following data:

- Gaseous species : Iodine.
- Source : 1 line source.
- Meteorological situations : 4 situations, rotating wind with an increasing speed (0.1m/s, 2m/s, 5m/s et 10m/s).
- Urban environment.

The simulation uses the following files:

- `puff.cfg` gives the simulation domain, options and the paths to the other files.
- `gaussian-levels.dat` gives the vertical levels.
- `gaussian-species_aer.dat` gives all meteorological data and scavenging and deposition coefficients. It was created during preprocessing (see Section 3).
- `puff-source-discretized.dat` gives data on the discretized source. It has been created using program `discretization` (see Section B.2).
- `puff-saver.cfg` gives the options and paths to save the results.

Compile the program `puff`:

```
cd ~/Polyphemus/driver/
make puff
```

Then execute it from `TestCase/`:

```
cd ~/TestCase/
~/Polyphemus/driver/puff config/puff.cfg
```

Results are stored in `results/puff_line/`.

B.4 Result Visualization

B.4.1 Gaussian Plume

Python scripts are provided to display easily and quickly the results of a simulation. For the plume simulation, just launch:

```
cd ~/TestCase/
python results/plume/display_plume.py
```

It creates 5 figures in `results/plume/`:

- `plume_gas_max` gives the repartition of the maximum of concentration of Iodine for all meteorological situations.
- `plume_gas_meteo1` gives the concentration for the first meteorological situation.
- `plume_gas_meteo2` gives the concentration for the second meteorological situation.
- `plume_gas_meteo3` gives the concentration for the third meteorological situation.
- `plume_gas_meteo4` gives the concentration for the fourth meteorological situation.

Figure B.1 shows the result of `display_plume.py`. Note that you can replace `Iodine.bin` with `Caesium.bin` in `results/plume/disp.cfg` to display the results for Caesium.

B.4.2 Gaussian Puff with Aerosol Species

Launch the python script to display the results:

```
cd ~/TestCase/
python results/puff_aer/display_puff.py
```

This creates 4 figures in `results/puff_aer/`:

- `puff_aer_meteo1` shows the puff at $t = 0s$, $t = 3s$ and $t = 8s$ for the first meteorological situation.
- `puff_aer_meteo2` shows the puff at $t = 0s$, $t = 3s$ and $t = 8s$ for the second meteorological situation.
- `puff_aer_meteo3` shows the puff at $t = 0s$, $t = 3s$ and $t = 8s$ for the third meteorological situation.
- `puff_aer_meteo4` shows the puff at $t = 0s$, $t = 3s$ and $t = 8s$ for the fourth meteorological situation.

Figure B.2 shows what is displayed. It shows how the puff evolves in time. By default, the species displayed is the first aerosol species and the first diameter class(`aer1_0`). Just modify the file `results/puff_aer/disp_puff.cfg` to display other species or diameters.

B.4.3 Gaussian Puff with Line Source

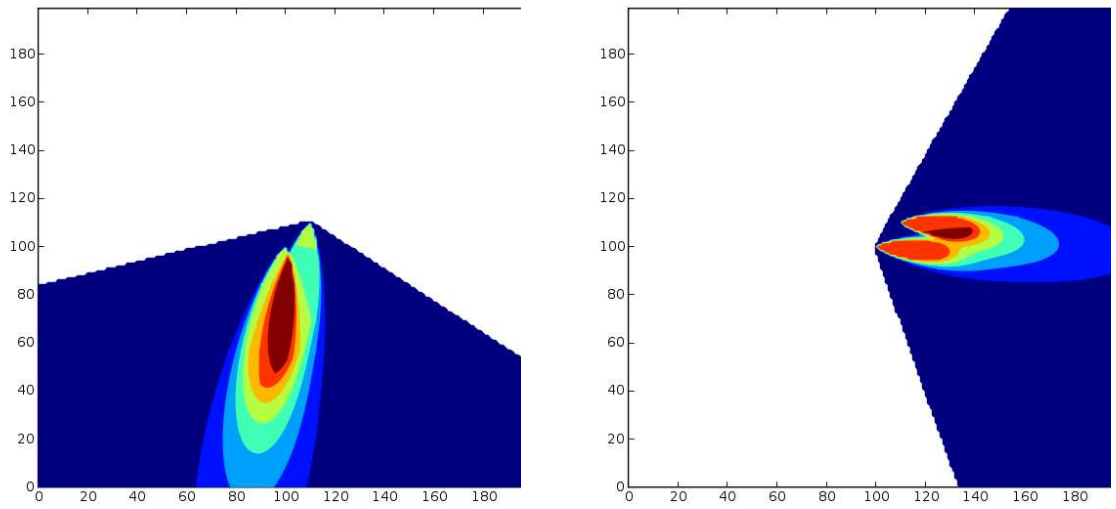
Launch the python script to display the results:

```
cd ~/TestCase/
python results/puff_line/display_puff.py
```

This create 4 figures in `results/puff_line/`:

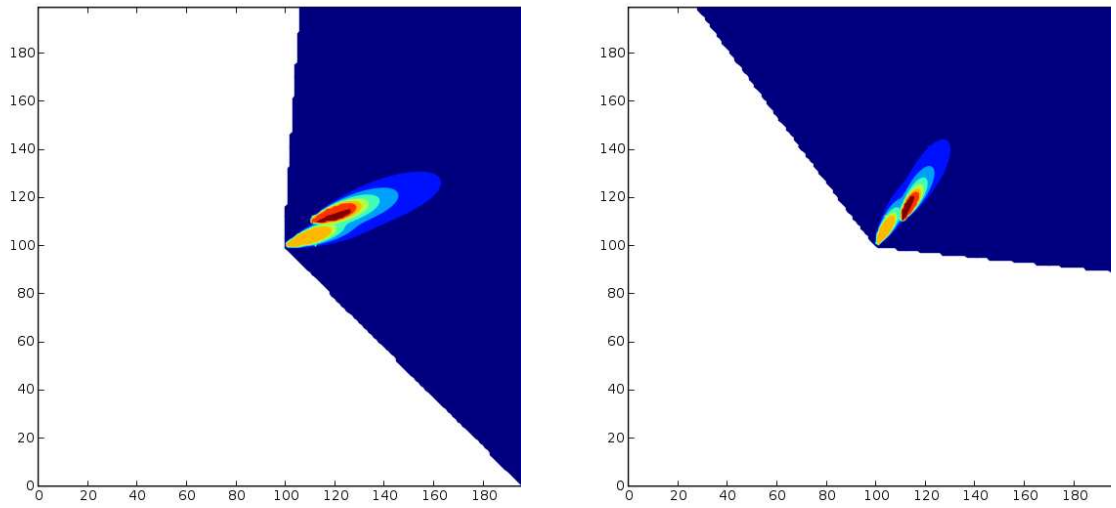
- `linepuff_meteo1` gives the concentration for the first meteorological situation.
- `linepuff_meteo2` gives the concentration for the second meteorological situation.
- `linepuff_meteo3` gives the concentration for the third meteorological situation.
- `linepuff_meteo4` gives the concentration for the fourth meteorological situation.

Concentrations are given for Iodine at t = 4s (middle of the simulation). Figure B.3 shows what is displayed.



(a) Situation 1

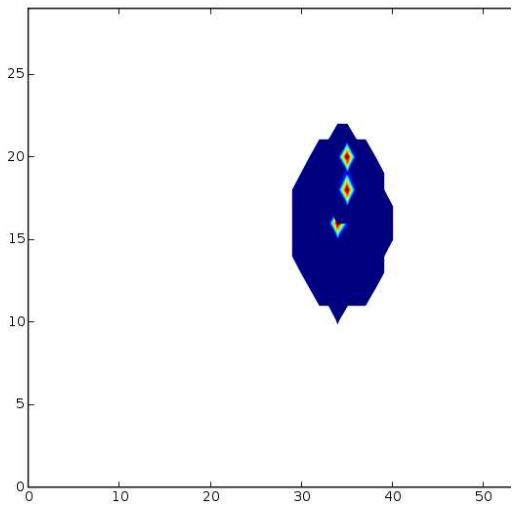
(b) Situation 2



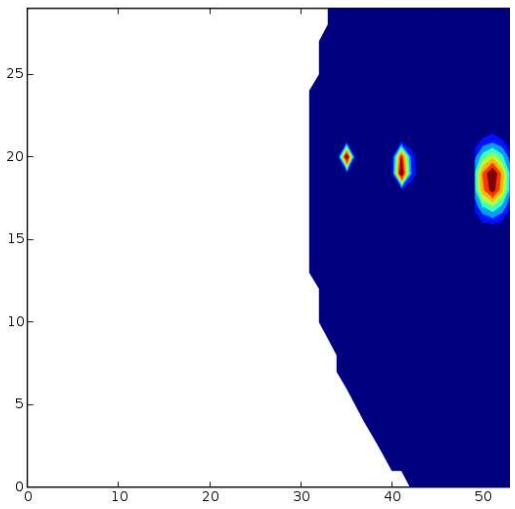
(c) Situation 3

(d) Situation 4

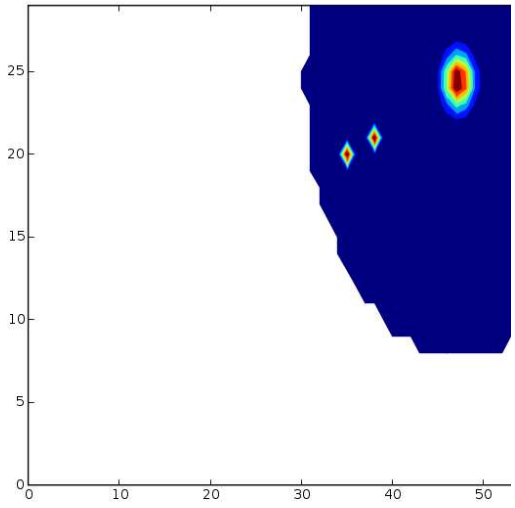
Figure B.1: Plume for the various meteorological situations.



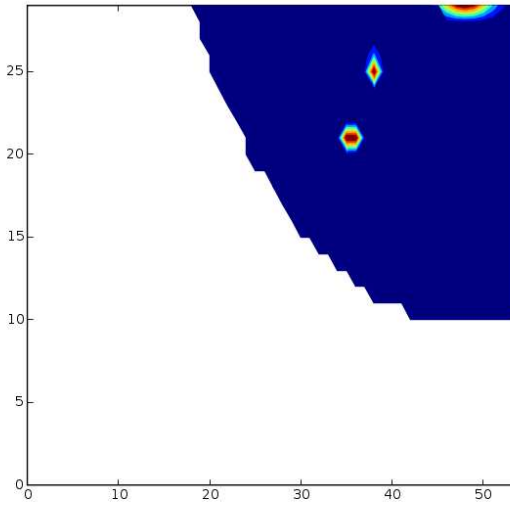
(a) Situation 1 - Concentration at $t = 0s$, $t = 3s$ and $t = 8s$



(b) Situation 2 - Concentration at $t = 0s$, $t = 3s$ and $t = 8s$

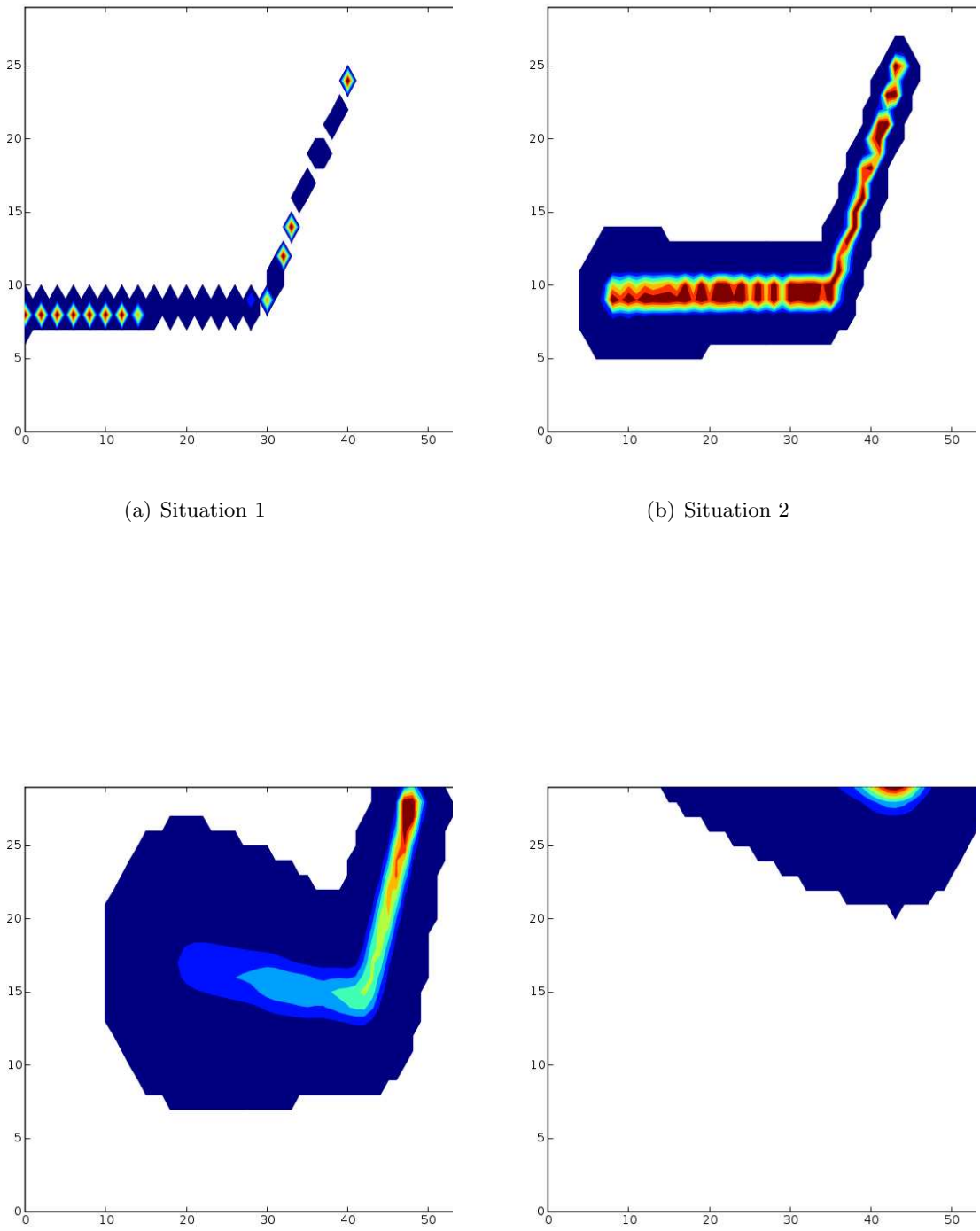


(c) Situation 3 - Concentration at $t = 0s$, $t = 0.5s$ and $t = 2.5s$



(d) Situation 4 - Concentration at $t = 0s$, $t = 0.5s$ and $t = 2.5s$

Figure B.2: Evolution of the puff for the various meteorological situations.



(a) Situation 1

(b) Situation 2

(c) Situation 3

(d) Situation 4

Figure B.3: Concentration at t = 4s for the various meteorological situations.

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